July 2017

Relationship Between Structure and Function in Nickel Proteins and Enzymes

Carolyn Carr

RELATIONSHIP BETWEEN STRUCTURE AND FUNCTION IN NICKEL PROTEINS AND ENZYMES

A Dissertation Presented

by

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Submitted to the Graduate School of the
University of Massachusetts Amherst in partial fulfillment
of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2017

Chemistry

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ACKNOWLEDGMENTS

First, and foremost, what would I have done without Heidi Hu. Heidi taught me most of what I know and everything I have forgotten. She was not only integral to my technical training, but also was the person with whom I had all my scientific discussions, which would eventually form the conclusions of this dissertation. My most heartfelt thanks go to Heidi.

Then there is my family to thank, specifically my mother, Margaret A. Thurn, J.D., for her continuous support throughout my life and for never trying to influence the course of my future with her own wishes, but being content to let me decide for myself.

Next, I acknowledge the help of Dr. Andrew Foster and Dr. Deenah Osman, postdocs in Dr. Nigel Robinson's group at Durham University, United Kingdom, who taught me both spectroscopic and biological techniques. In addition, I thank Dr. Peter Chivers for bestowing our lab with ΔRcnR *E. coli* cells and for teaching me to perform β-galactosidase experiments.

I also thank Dr. Diane Cabelli for her aid with pulse radiolysis and her stimulating discussion of NiSOD; Dr. Cornelius Taabazuing for teaching me how to do EPR; and Keith Lehuta for helping me perform quantitative EPR. In addition, I would like to acknowledge the beamline scientists at both NSLS and SSRL for their help in data collection.

Last, but not least, my recognition of the graduate students at UMass Amherst, not just in the Chemistry Department but also those in or affiliated with the MCB and CBI programs. There was never a single graduate student I met at UMass Amherst who was not friendly and helpful.

ABSTRACT

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MAY 2017

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Nickel is a rarely used but biologically important metal that is utilized in all three domains of life. In nickel utilizing organisms there is a corresponding trafficking system specifically designed to capture nickel, deliver, and export excess nickel to prevent toxic effects. It is critical to understand the mechanisms by which organisms achieve metal selectivity to duplicate or disrupt this process for the benefit of human health and to further understanding of regulation mechanisms in biology.

RcnR is a Ni(II) and Co(II) responsive transcriptional regulator in *E. coli*. The research reported in this dissertation focuses on the relationship between structure and function in two hypothesized metal ligand residues, Glu34 and Glu63. The results of these studies indicate that Glu34 is a Co(II) ligand and Glu63 is both a Ni(II) and Co(II) ligand. It is clear from the results of these studies that there is little correlation between metal structure and function in RcnR, and that studies of metal site structure or function alone cannot be used to determine metal response or residue importance. It is clear from analysis of this family of transcriptional regulators that although homologous, they have divergent mechanisms.

Reactive oxygen species (ROS) are a natural byproduct of aerobic metabolism and inflammation, and can be generated through environmental factors such as radiation damage, pollution, and smoking. ROS such as superoxide can cause damage to DNA, lipids, and proteins if left unchecked. Superoxide dismutases are a family of enzymes that catalyze the disproportionation of superoxide to prevent its harmful effects. One of the goals of this dissertation is to investigate how NiSOD exerts control over the redox state of the nickel centers.

NiSOD is a hexamer that cannot be fully oxidized and thus remains 50% Ni(II)/50% Ni(III). One possible reason this occurs is by crosstalk of the nickel centers through a hydrogen bonding network involving His53. Disruption of this crosstalk was attempted by mutation of His53 to alanine. While the experimental evidence indicates the mutation did not disrupt the crosstalk, it is apparent that the entire ~ 40 Å hydrogen bonding network is important for modulating the catalytic mechanism.

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ATP	Adenosine Triphosphate
ATPase	Adenosine Triphosphatase
JMJD1A	Jumanji domain 1A
JMJD2	Jumonji domain 2
ABH2	AlkB homolog 2
ABH3	AlkB homolog 3
PHD2	Prolyl Hydroxylase domain protein 2
HIF1α	Hypoxia Inducible Factor 1α
E. coli	*Escherichia coli*
InrS	Internal Nickel Responsive Sensor
ABC transporter	ATP-binding Cassette Transporter
TMD	Transmembrane Domain
NBD	Nucleotide Binding Domain
NikR	Nickel Responsive Regulator
CorA	Cobalt/magnesium Transport Protein
FNR	Fumarate and Nitrate Reduction Regulatory Protein
RcnA	Resistance to Cobalt and Nickel A
RcnR	Resistance to Cobalt and Nickel Regulator
RcnB	Resistance to Cobalt and Nickel B
FHL	Formate Hydrogen Lyase
ArsR	Arsenic Repressor
SmtB	*Synechococcus* Metallothionein
MerR	Mercury Responsive Transcriptional Regulator
CopY	Copper Responsive Regulator

Fur	Ferric Uptake Regulation Protein
DtxR	Diptheria Toxin Repressor
CsoR	Copper-sensing Transcriptional Regulator
C. glutamicum	*Corynebacterium glutamicum*
L. monocytogenes	*Listeria monocytogenes*
D. radiodurans (Dr)	*Deinococcus radiodurans*
S. lividans	*Streptomyces lividans*
T. thermophilus (Tt)	*Thermus thermophilus*
FrmR	Formaldehyde Responsive Regulator
CstR	CsoR-like Transcriptional Regulator
RicR	Regulated in Copper Repressor
DmeR	Divalent Metal Efflux Regulator
NcrB	Nickel Resistance Determinant B
Amp	Ampicillin
Cam	Chloramphenicol
IPTG	Isopropyl β-D-1-thiogalactopyranoside
TCEP	Tris(2-carboxyethyl)-phosphine hydrochloride
PMSF	Phenylmethyl-sulfonylfluoride
HEPES	4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid
Tris	2-Amino-2-hydroxymethyl-propane-1,3-diol
EDTA	Ethylenediaminetetraacetic acid
ESI-MS	Electrospray Ionization Mass Spectrometry
XAS	X-ray Absorption Spectroscopy
EXAFS	Extended X-ray Absorption Fine Structure

ICP-OES	Inductively Couple Plasma-Optical Emission Spectroscopy
NSLS	National Synchrotron Light Source
SSRL	Stanford Synchrotron Radiation Lightsource
XANES	X-ray Absorption Near Edge Spectroscopy
ONPG	*o*-nitrophenyl-β-D-galactopyranosidase
OD	Optical Density
5'-TAMRA	5-carboxytetramethylrhodamine
ROS	Reactive Oxygen Species
SOD's	Superoxide Dismutase
MnSOD	Manganese Superoxide Dismutase
FeSOD	Iron Superoxide Dismutase
CuZnSOD	Copper Zinc Superoxide Dismutase
NiSOD	Nickel Superoxide Dismutase
NO	Nitric Oxide
CCS	Copper Chaperon for Superoxide Dismutase
C. elegans	*Caenorhabditis elegans*
NHE	Normal Hydrogen Electrode
SUMO	Small Ubiquitin-Related Modifier
Ulp1	Ubiquitin-Like Specific Protease 1

CHAPTER 1

MAINTENANCE OF CELLULAR METAL HOMEOSTASIS BY METALLOREGULATORS

1.1 Metals in Biology

It has been estimated that at least one-third to one-half of all proteins require metal in order to perform their function.[1–3] Metal containing proteins are required for some of life's most important processes, such as the manganese cluster in Photosystem II[4] and the three iron-sulfur clusters in Photosystem I,[5] which are involved in the photosynthetic process of plants. Metals are also important for a wide variety of critical functions in humans, ranging from the heme cofactor, which binds oxygen in hemoglobin, to the two copper centers in cytochrome c oxidase, which catalyze the conversion of oxygen into water, thereby facilitating the maintenance of the proton electrochemical gradient within the mitochondria that drives ATP synthesis.[6] These few examples of the biological uses of metals show that being deficient in even one type of metal can have a severe impact on the health of a cell. Chronic or hereditary deficiency, such as in the case of Menkes disease, which is caused by a defective Cu-transporting ATPase, can lead to severe neurodegeneration, bone loss, and deterioration of the nervous system.[7–9] While it is obvious that metals are of critical importance, their presence within the cell can also be detrimental if not regulated. Metals such as iron or copper can react with DNA, lipids, and protein and generate free radicals, such as in the case of excess iron in people with hereditary haemochromatosis[10–13] or excess copper in Wilson's disease.[7–9] This can lead to a large variety of effects, as this damage is non-specific. Excess metals can also cause very specific damage, such as in the case of zinc,

which causes copper deficiency,[14–18] and cobalt which impairs iron sulfur cluster synthesis.[19–22] Thus, metal ion homeostasis is imperative for the survival of the cell.

1.2 Nickel and Cobalt Toxicity

Nickel and cobalt are trace metals which lack the appeal of readily accessible redox chemistry of iron or copper, but are still capable of redox chemistry with appropriate tuning, unlike zinc. While there are no known nickel binding proteins in mammals, both metals are used in prokaryotes and archaea as essential cofactors for an astonishing range of biological processes. There are currently nine known nickel containing enzymes; glyoxalase I, acireductone dioxygenase, nickel containing superoxide dismutase, urease, NiFe-hydrogenase, acetyl-coenzyme A synthase, carbon monoxide dehydrogenase, methyl-coenyzme M reductase, and recently lactate racemase.[23–26] Cobalt ions are catalytically relevant cofactors in a variety of proteins including, but not limited to, *Salmonella typhimonium* methionine aminopeptidase, *Rhodococcus rhodochrous* nitrile hydratase, *Pyrococcus furiosus* prolidase, *Propionibacterium shermanii* methylmalonyl-coenzyme A carboxytransferase, and *Pseudomonas putida* bromoperoxidase.[27,28] In nearly all of these proteins, cobalt is only one of several metals (Zn(II), Fe(II), Cu(II)) that produce a functionally active protein. In addition to these proteins utilizing cobalt ions as cofactors, a large variety of proteins utilize vitamin B_{12} and cobalamins as essential cofactors.[28,29] Animals and many prokaryotes including *Escherichia coli* cannot synthesize their own B_{12} or cobalamins and thus must obtain these from their environment by transporting the intact vitamin using a porphyrin transport system.[29–31]

Whether a cell utilizes a specific metal does not abolish the toxic effects of the metal at high concentrations. Both nickel[32–35] and cobalt[36–40] ions have been shown to cause neurodegenerative disorders, inflammation, and cancer in humans. However, the tolerance to cobalt toxicity may be higher in humans due to the use of cobalamins while there is still no evidence of nickel utilization. A large body of research has been performed on mice, rats, and primates regarding the genotoxic and respiratory toxicity of nickel, and efforts have been made to correlate this with the epidemiology of cancer risks to workers in nickel refineries.[32] Extensive animal carcinogenicity studies indicate that nickel ions themselves are not carcinogenic (**Figure 1.1**), with soluble nickel compounds and metallic nickel having low carcinogenic properties. On the other hand, insoluble

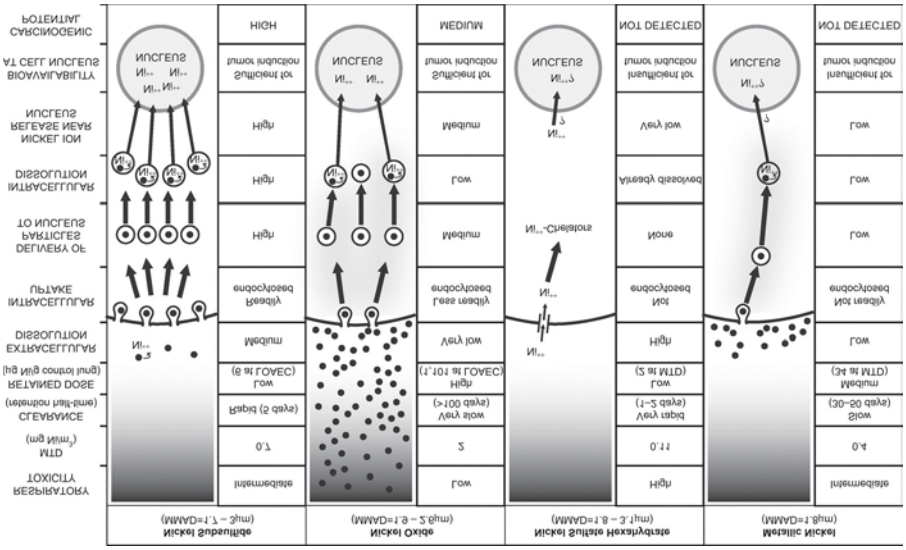

Figure 1.1: A highlight of the key features of the nickel ion bioavailability model that takes into account the various factors that determine the bioavailability of the nickel ion at the nucleus of target cells *in vivo*. The examples in this figure are based on the results of *in vitro* and *in vivo* mechanistic studies. Reproduced with permission from ref 32. MMAD, mass median aerodynamic diameter; MTD, maximum tolerated dose; LOAEC, lowest observable adverse effect concentration.

nickel compounds significantly increase the occurrence of cancer in mice, rats and primates.[32] However, this does not correlate well with studies of the epidemiology of workers in nickel refineries, where the total amount of nickel exposure was a clear

indicator of cancer risks experienced by the workers. While current data states that soluble and metallic nickel compounds alone do not strongly increase the risk of cancer, that is not to say that soluble nickel compounds alone are not dangerous, as they have low carcinogenicity but high risk for respiratory toxicity, causing increased inflammation and cytotoxicity.[32]

The difference in toxicity is partly attributed to the method of intake, with soluble nickel compounds being cleared quickly from the extracellular matrix due to its respiratory toxicity and entering cells via ion channels in small quantities, too small to enter the nucleus in any significant amount.[32,34,41] This is in direct contrast to sulfidic nickel, which has the highest carcinogenic properties. Sulfidic nickel compounds have intermediate clearance rates possibly due to its lack of respiratory toxicity but are the most readily taken up via endocytosis. Specifically, crystalline compounds whose overall surface charge is negative are taken up, as opposed to positively charged amorphous sulfidic nickel.[32,34,41] The insoluble nickel is then dissolved in the acidic environment of the endosome, and through a yet unknown mechanism is trafficked to the nucleus.[32,41] There is some evidence that endosomes containing nickel particles interact with liposomes with a higher frequency, facilitating nickel particle dissolution. Soluble nickel compounds remain almost entirely within the cytoplasm, but in one study nickel chloride packaged in liposomes were subjected to endocytosis, and this yielded an increase in cellular nickel uptake and heterochromatin damage, indicating that entry into the nucleus via endocytosis is key to understanding the status of different carcinogenic nickel compounds.[32]

Previous research on the reason for nickel targeting of heterochromatin specifically and its carcinogenic effect on the cell found that nickel readily substitutes for the native magnesium ions that surround and compact chromatin.[41] Nickel binds tighter than magnesium and is much better at compacting the structure. This compaction causes euchromatin to be methylated and drawn into heterochromatin, leading to gene silencing.[41]

One of the key features of nickel toxicity in mammalian cells is disruption of iron homeostasis, through a combination of disruption of iron import in transferrin dependent and independent pathways[35] and nickel substitution in the active site of a variety of enzymes. While the mechanism for iron depletion is unknown, it has been well documented that Ni(II) inhibits the iron and α-ketoglutarate dependent dioxygenase family of enzymes, which bind the active site iron via a His/His/Asp facial triad.[42,43] This causes inhibition in a wide range of critical enzymes, including histone demethylases such as JMJD1A and JMJD2, DNA repair nucleotide demethylases such as ABH2 and ABH3, and oxygen-sensing prolyl hydroxylases such as PHD2.[35] It has been shown that nickel binds the active site of these enzymes with a ~3 fold increase in affinity compared to iron, and the nickel center adopts a six-coordinate geometry as opposed to the 5-coordinate geometry of iron, which allows oxygen to bind.[42,43] Inhibition of DNA-modifying enzymes such as ABH2 and JMJD2 would lead to gene silencing and epigenetic effects, which help explain the carcinogenic effect of nickel toxicity. Inhibition of enzymes like PHD2 leads to activation and stabilization of HIF1α, which in turn induces HIF1α dependent genes. Current *in vivo* data shows an accumulation of HIF1α in cells exposed to nickel, which not only leads to HIF1α gene induction, but it

has been shown that HIF1α competes with tumor suppressor protein p53 for the co-activator protein p300.[44] While p53 itself is upregulated in nickel exposed cells, the genes under its control are not upregulated, which has been attributed to the high levels of HIF1α competing with p53 for p300. This would lead to upregulation of genes involved in cell proliferation and angiogenesis but steady state or downregulation of tumor suppression genes.

In contrast to nickel, whose toxicity in soluble form is minimal and not considered a major risk factor, soluble cobalt is considered the primary toxic species. Thus, there is little consideration of the effects of cobalt mining on the miners. Instead, there is currently a concern for people with prosthetics, which typically contain high levels of cobalt that corrode in the body and produce soluble cobalt species.[38] Soluble cobalt is known to cause generalized oxidative damage through the Fenton reaction, the same as many other heavy metals that enter the body.[20,22,37,38,40] However cobalt has more specialized effects, specifically on iron proteins with evidence that cobalt effects FeS cluster synthesis.[20–22,40] It does not affect clusters in fully folded and functional proteins, but specifically targets labile clusters in scaffold proteins.[22] In addition, cobalt appears to have the same effect on HIF1α as nickel, leading to the upregulation of genes involved in cell proliferation and downregulation of tumor suppression genes, supposedly by replacing the active site iron with cobalt.[44] This is related with the previous medical use of cobalt for treatment of anemia, due to the ability of cobalt to massively induce the production of red blood cells (leading to polycythemia in healthy people). This presumably works because cobalt replaces the iron in hemoglobin, resulting in the body responding as if it is oxygen deficient.[38,45,46]

While there is currently a plethora of literature on the health effects of heavy metals on humans and environmental wildlife, literature investigating the toxic effects of heavy metals on bacteria is sparse. However, understanding how proteins achieve selectivity for all metals is becoming more critical as concerns rise due to the increasing addition of metals to consumer products for antimicrobial purposes, and the increasing development of multi-drug resistant pathogens.[47] Because humans do not have any known nickel-requiring proteins, understanding how nickel-requiring bacterial proteins select for nickel and how excess nickel induces toxicological effects in bacteria is of critical importance for development of potent antimicrobial nickel compounds that will not interfere with any human biological processes while simultaneously being effective as antimicrobial agents.

1.3 Nickel Trafficking in *E. coli*.

The nickel trafficking system in *E. coli* is an optimal system to study to learn how trafficking proteins select for their cognate metals. All of the major components have been identified and have been shown to be functionally specific for only their cognate metal, which is not the case for members in other trafficking systems (see section 1.4.3). The reason for the simplicity of this system is that there is only one target enzyme for this pathway that requires nickel for function, i.e., NiFe-hydrogenase. NiFe-hydrogenase carries out the oxidation of hydrogen to protons and electrons, a reaction that is reversible depending on the isoform.

1.3.1 Nickel Uptake and Export

The ABC transporter NikABCDE facilitates nickel entry into the cell. This importer is encoded by the *nik* operon[48] and contains a periplasmic Ni-(L-His)$_2$ binding

protein, NikA, that binds the enantiomer specific complex though hydrogen and ionic bonds and through direct axial coordination of His416[49] to the Ni(II). NikA then delivers it to the membrane components of the ABC transporter, NikB and NikC.[49–51] NikB and NikC are the canonical transmembrane domains (TMDs) common to all ABC transporters, which translocate the substrate from the periplasm to the cytoplasm.[52] NikD and NikE are the two canonical nucleotide binding domains (NBDs) and are highly conserved, unlike the TMDs.[52] The NBDs bind and hydrolyze ATP, which provides the energy for unidirectional substrate transport through the TMDs NikB and NikC.[53,54] In addition to this highly specific Ni(II) importer, Ni(II) can also enter the cell through other nonspecific divalent metal transporters such as CorA, which is the primary Mg(II) importer in *E. coli*.[55] There may be a high number of nonspecific divalent transporters due to the fact that in CorA and NikABCDE deletion strains of *E. coli*, NikR still represses transcription of NikABCDE, indicating Ni(II) import into the cell.[56] Deletion of NikABCDE abolishes hydrogenase activity, which can be recovered by addition of excess nickel to the growth medium.[57,58]

nikABCDE is upregulated by FNR, which is activated under low oxygen conditions in a nickel independent manner, and downregulated by NikR in the presence of nickel.[58] Excess nickel increases the binding of NikR further, overriding FNR to repress *nikABCDE*.[50] In addition to regulating the *nik* operon, FNR is also responsible for partial control of *nikR*.[59] It was found that NikR can bind a wide variety of transition metals with an affinity that reflects the Irving-Williams series: k_a: Mn(II)<Co(II)<Ni(II)<Cu(II)>Zn(II). But in terms of protein stability, Ni(II) has the greatest effect.[60] Adding stoichiometric amounts of most transition metals induces

binding to the *nik* operon, but not to the same degree as nickel.[61] Adding excessive nickel strongly induces protein stabilization, indicating that there is more than one nickel binding site, which have since been termed the high-affinity and low-affinity nickel sites.[59,61] Protein digestion experiments revealed that Ni(II) and Cu(II) induce a conformation different than apo-NikR, although the change with Cu(II) is much weaker.[62] Co(II) and Zn(II) do not change the conformation at all. H/D exchange experiments done by others lead to conclusions regarding protein conformation that are identical to the protein digestion experiments, where Ni(II) and Cu(II) induce a similar conformation upon binding to NikR, but with Cu(II) to a much less extent than Ni(II), while Co(II) and Zn(II) adopt an apo-NikR conformation.[63] A crystal structure of NikR implicated the presence of potassium ions bound to NikR.[64] Molecular simulations were done to provide a basis for this, and found that for the high affinity site, nickel is the preferred metal with potassium causing conformational changes that disfavor ion binding.[65] Although the free binding energy of Ni(II) and K+ to the low affinity site are equal, K+ is considered the cognate metal for this site as there is a desolvation penalty associated with Ni(II). Mobility shift assays and DNase foot-printing reveal that in the absence of any potassium, NikR does not bind to DNA and with the addition of excess Ni(II), the DNA binding is enhanced.[66] This is indicative of not only two Ni(II) sites of varying affinities, but also evidence for potassium binding sites. This is a more probable explanation for the 22 binding sites attributed to low affinity Ni(II) binding sites identified in a NikR crystal structure obtained from crystals soaked in $NiCl_2$.[67]

RcnA is a periplasmic protein whose deletion causes growth inhibition and whose overexpression causes enhanced resistance to both nickel and cobalt.[68] Deletion causes

nickel and cobalt accumulation in cells.[68] In a similar vein to NikABCDE, RcnA was shown to be regulated by both RcnR, a Ni(II) and Co(II) responsive regulator, and Fur, which is an iron dependent regulator.[69] RcnA belongs to a new family of exporter proteins, and its rate of export was recently shown to be modulated by another protein in the *rcn* operon, RcnB. RcnB is a periplasmic protein that does not appear to bind Ni(II) or Co(II) directly but interacts with RcnA in a way to reduce efflux.[70]

RcnR is the other nickel responsive transcriptional regulator present in *E. coli* and controls expression of the *rcn* operon which consists of RcnA and RcnB as well as RcnR itself so that RcnR controls its own expression.[71] Similar to RcnA, RcnR is responsive to both Ni(II) and Co(II) *in vivo* but is not responsive to other transition metals.[72] Apo-RcnR is bound to DNA and upon the binding of nickel or cobalt, for which it has a K_d in the nanomolar range, a conformational change is induced, which disfavors DNA binding, allowing for transcription of RcnA/B.

1.3.2 NiFe-Hydrogenase and Its Metallochaperones

In addition to preventing toxicity due to excess nickel, the nickel trafficking system in *E. coli* acquires nickel for the maturation of [NiFe]-hydrogenase, of which *E. coli* has three isoforms.[73] A fourth set of hydrogenase genes (*hyf* operon) have been discovered. However, no *hyf* encoded proteins or *hyf* dependent H_2 evolution was measured, so its function is still unknown.[74] The other three isoforms allow *E. coli* to generate energy under three alternative environments: aerobic respiration by the oxygen tolerant hydrogenase-1 (*hya* operon), anaerobic respiration by the bidirectional oxygen-intolerant hydrogenase-2 (*hyb* operon), and fermentation by hydrogenase-3 (*hyc* operon),

which is part of the formate hydrogenlyase (FHL) system and reduces the protons generated from the formate dehydrogenase reaction to dihydrogen.[75]

Each [NiFe]-hydrogenase has two sets of maturation genes. Group 1 is located on the same transcription unit as the structural genes. Disruption of the Group 1 maturation genes specifically impairs the processing or maturation of the structural genes located on the same transcription unit. The only exception to this rule is *E. coli* HybG which is located on the hydrogenase-2 subunit but is involved in the maturation of both hydrogenase-1 and 2.[76] Disruption of these genes cannot be complemented by homologous genes from other transcripts, supposedly due to highly specific protein-protein interactions.[77] The second set of genes is the *hyp* (hydrogenase pleiotropic) genes that affect all hydrogenases. *E. coli* has only one set of *hyp* genes except for *hypC*, which is not involved in hydrogenase-2 maturation (replaced by *hybG*), and *hypA*, which is only involved in hydrogenase-3 (hydrogenase-1 and 2 utilize *hybF*) maturation. *Hyp* proteins can be complemented by heterologous genes from other organisms.[78]

The first step in the maturation of a [NiFe]-hydrogenase is complex formation between HypC and the large subunit precursor before active site ($NiFe(CN)_2CO$) formation. HypC deletions lead to Ni free hydrogenase, indicating complex formation before active site insertion.[79] In addition, the C-terminal extension is required for precursor association with HypC, and cleavage of this extension occurs immediately after active site assembly and insertion.[80] Hydrogenase cysteines that bind the Ni are involved in HypC-preHycE (hydrogenase-3 terminology) formation, so HypC keeps hydrogenase in a metal accessible conformation.[81]

Once a HypC-preHycE complex forms, HypC then forms a complex with HypD, which has been proposed to contain the active site Fe atom, and this HypD/HypC/preHycE complex interacts with a HypF/HypE complex, both of which are absolutely required for maturation[82,83] and which synthesize the cyanide ligand from carbamoylphosphate.[84] HybF converts carbamoylphosphate to carbamoyladenylate before transferring the carbamoyl group to the C-terminal cysteine of HypE.[85,86] This thiocarboxamide group is then converted to thiocyanate and transferred from HypE to an Fe ion in the HypC/D complex.[86,87] Complexation of HypC/D is required for transfer, no transfer occurs with the individual components.[88]

HypA and HypB are involved in Ni insertion into [NiFe]-hydrogenase but are not absolutely required because Ni addition to the medium restores hydrogenase activity.[89] Ni insertion occurs only after the Fe complex is inserted into the active site.[90] HypA is a metallochaperone that exists in both monomeric and dimeric states and coordinates Ni via an N-terminal MHE motif and Zn through a Zn-finger motif.[91] HypA exhibits low sequence conservation outside the Ni and Zn motifs, which mirrors the diversity of both HypBs and [NiFe]-hydrogenases.[92] HypB is a metallochaperone with GTPase activity that is required for hydrogenase maturation.[93,94] All HypBs have a low affinity metal site in the GTPase domain that binds both Ni and Zn but a select few have a high affinity N-terminal nickel binding site with a CxxCGC motif.[95,96] HypB has been shown to form a complex with pre-HycE (hydrogenase-3 large subunit precursor) only with HypA present.[97] There is a third metallochaperone whose gene is not located on either the *hyb* or *hyp* operon and which is not involved in the maturation of hydrogenases in all organisms. SlyD is an FKBP prolyl isomerase that has both an isomerase domain and a

hydrophobic chaperone domain. A subset of SlyD contain an unstructured C-terminal tail that has a high cysteine/histidine content. The current proposed mechanism in *E. coli* is that metallochaperone SlyD delivers Ni via an unstructured C-terminal metal binding tail to HypB which dimerizes and then interacts with HypA and pre-HycE for Ni delivery.[97–99]

The last maturation step is proteolytic cleavage of the C-terminus, which occurs after HypC dissociation from the large subunit.[81] Each hydrogenase has its own endopeptidase that cleaves after a conserved His or Arg in a CxxCxxH/R motif,[90,100] and amino acid substitutions at or near the cleavage site lead to maturation abortion.[100,101] The presence of Ni in the active site is absolutely required for C-terminal cleavage.[90,102]

1.4 RcnR/CsoR Family of Transcriptional Regulators

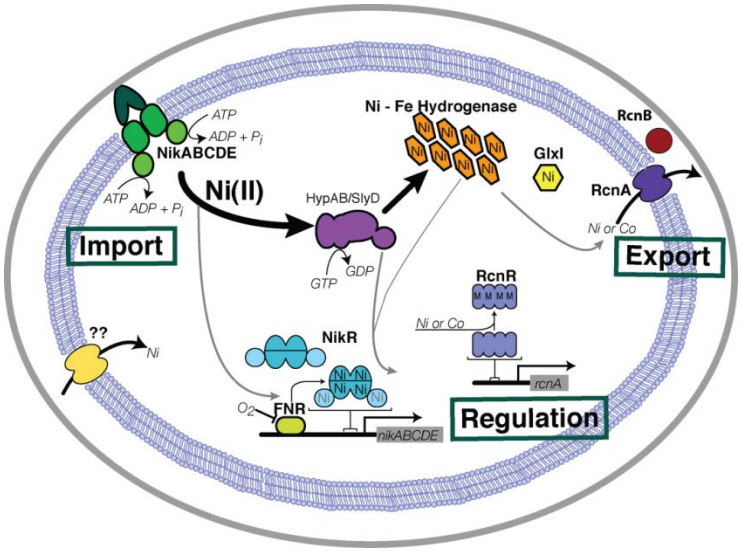

Figure 1.2: Schematic of the nickel trafficking system in *E. coli*. Reprinted with permission from Ref. 102. Copyright 2012 American Chemical Society.

For a cell to maintain homeostasis it must have a fully functional transport system. A basic transport system needs to allow for metal specific entry and exit (importer and exporter proteins), proteins that will then deliver the specific metal to its necessary destination (metallochaperones), and finally proteins that regulate the other members of the trafficking pathway (metalloregulators) (Figure 2).[103] Proteins within a trafficking pathway must be specific for their intended metal ion, as excessive incorporation of, for instance, zinc into copper trafficking proteins would then lead to copper deficiency despite fully functional copper transport proteins.[14–18] The method of ensuring specificity varies depending on the organism. However, trafficking proteins must also be able to release their metal ion so that it can be delivered to its target or removed from the cell.

Accordingly, for a cell to efficiently respond to the intracellular level of metal ions by either enhancing uptake or efflux, the metalloregulators must be able to detect the varying metal levels inside the cell. Metalloregulators response to the binding of transition metals subsequently favors or disfavors its interaction with DNA, which ultimately leads to expression or repression of the genes under its control. There are currently seven major families of transcriptional regulators that contain metal responsive regulators: ArsR/SmtB,[104,105] MerR,[106] CsoR/RcnR,[107–109] CopY,[110–112] Fur,[113,114] DtxR,[115–117] and NikR.[118] These families are differentiated by their overall protein fold. Although many of these metalloregulators bind a variety of metals *in vitro*, *in vivo* these regulators either respond only to their cognate metals or the intracellular concentration of metals is such that only their cognate metal induces the allosteric change necessary to alter DNA affinity.

1.4.1 CsoR

CsoR is the most well studied member of the CsoR/RcnR family of metalloregulators and is a perfect example of the diversity seen in the rest of the family. In all organisms where the genes under CsoR control have been confirmed, CsoR at minimum controls the expression of one set of the copper efflux P1-type ATPase, CopA, and the copper chaperone CopZ (**Table 1.1**). In *C. glutamicum*, which contains two sets of CopZ genes located in different operons, it has been shown that the two CopZ genes are redundant, with growth defects being observed only with deletion of both CopZ genes.[119,120] However, there is no growth defect after deletion of CopZ in other organisms (*L. monocytogenes, D. radiodurans).*[121,122] This is indicative of either a difference in the CopZ function or the presence of unidentified operons under the control of CsoR. As CopZ in *L. monocytogenes* delivers Cu(I) to CopA,[121,122] and CopZ from *S. lividans* delivers Cu(I) to CsoR,[123] both hypotheses are possible. CsoR does not have a true consensus sequence, and features widely divergent DNA sequences across different species. The RcnR/CsoR family has been separated into seven different clades based on amino acid sequence with CsoR present in four out of seven clades.[124] In some cases these clades correspond to similar DNA-binding sequences (*Thermus thermophilus*[125] and *Mycobacterium tuberculosis*[107]), but divergent sequences in others (*Listeria monocytogenes*[122] and *Bacillus subtilis*[126–129]*).* As the phylogentic tree was not comprehensive in its inclusion of studied CsoRs, and with more being identified, the addition of CsoRs from more organisms may change the distribution of CsoRs into different clades. Interestingly, *Tt*CsoR and *Dr*CsoR do not contain the typical C-H-C Cu(I) binding motif the other CsoRs contain, instead having a C-H-H motif.[121,125] These

two CsoRs are not contained in the same clade, and *Tt*CsoR in particular has been shown to be highly promiscuous *in vitro*, responding to Cu(I), Cu(II), Ni(II), Ag(I), Co(II), Zn(II) and Cd(II).[125] No metals were tested other than Cu(I) for *Dr*CsoR.[121] CsoR in *L. monocytogenes* was shown to not release from DNA upon the addition of Cu(I), only to change conformation which facilitates transcription.[122] This mechanism of transcriptional control has not been observed for CsoRs in other organisms. CsoR is most commonly interpreted to bind as a 'sandwich' with one CsoR on each face of the DNA. However, this has only been confirmed in *S. lividans*[130] and is unlikely to be a general mechanism based on the high dissimilarity in the amino acid (25% identity with CsoRs not in the same clade) and DNA-binding sequences of different CsoRs.

Table 1.1: The organisms in which CsoR has been identified, the genes under its control, the consensus sequence it binds to and the clade it was separated into based on Ref. 124.

Organism	Genes	DNA-sequence	Clade[124]
Staphylococcus aureus (Sau)[131]	copAZ, copBmco	Unknown	V
Listeria monocytogenes (Lm)[122]	copAZ	TATA-G_5-TATA	IV
Thermus thermophilus (Tt)[125]	copAZ	TA-C_4-A-C_4-ACCT-G_4-T-G_4-TA	I
Deinococcus radiodurans (Dr)[121]	copAZ + 2 ORF's	ACCAT-C_6-GGAGAGGGT	NA
Desulfosporosinus sp. OT *(Ds)*[132]	copAZ	TATA-G_6-TATA	NA
Corynebacterium glutamicum (Cg)[119,120]	copA, copBZ + 1 ORF, copZ2	ATA-C_4-ATA-G_4-TAT	III
Streptomyces lividans (Sl)[123,130,133]	3 copAZ	TA-C_4-TGGT-G_3-TA	III
Mycobacterium tuberculosis (Mt)[107,134]	3 ORF's	G-C_3-A-C_5-AGT-G_4-T-G_3-A	I
Geobacillus thermodentrificans (Gt)[124,135,136]	Unknown	TA-C_5-TTC-G_3-TA	IV
Bacillus subtilis (Bs)[126–129,137]	copAZ	TA-C_3-TAC-G_5-TA	IV

1.4.2 RcnR

RcnR controls the expression of the Ni(II) and Co(II) exporter proteins RcnA and RcnB.[68,70] Apo-RcnR responds to the binding of Ni(II) and Co(II) by undergoing a conformational change that disfavors DNA binding, allowing for transcription.[72] Induction of *rcnA* by RcnR only occurs when *nikR* expression is maximally inhibited.[71]

rcnA expression is also regulated by Fur, which has a consensus sequence in the *rcnR-rcnA* intergenic region, and this regulation is independent of RcnR.[69] Ni(II) and Co(II) bind to RcnR in sites with octahedral geometry, with both metals bound with a N/O_5S ligand set with the sulfur belonging to the single cysteine in the protein, Cys35.[72] Ni(II) was shown to bind the N-terminus, Cys35, and His64 while Co(II) was shown to additionally bind His3, revealing that, although RcnR responds to both metals, it binds them with slightly different ligand sets.[138,139] Both ligand sets propagate the signal of metal binding through the protein, leading to DNA release. The binding of Ni(II) and Co(II) does not impart major changes to the secondary or quaternary structure, but does increase protein stability.[72] DNase footprinting showed that RcnR strongly protects 41-42 bases, which include two G-tracts of 6-7 guanines that are flanked by TACT invert repeats.[140] Mutation of the G-tract or the TACT invert repeats causes a decrease in affinity.[140] Outside of these sites, there are hypersensitive sites every 10 bp for 60 bp on either side possibly due to DNA bending or wrapping.[140] One RcnR tetramer binds to each G-tract, but without both sites there are no hypersensitive sites or wrapping.[140] RcnR interacts with ~150 bp that extend into the coding regions of RcnR and RcnA.[140] In line with this extended DNA interaction, RcnRs DNA affinity increases by 4-fold when binding to 150 base pairs as opposed to 80 bp.[140] RcnRs interaction with DNA causes a single negative supercoil, and the G-tracts induce A-form rather than B-form DNA structure.[140]

1.4.3 InrS

InrS is a Ni(II) responsive transcriptional regulator in *Synechocystis* that controls the expression of the Ni(II) exporter *nrsD*.[141,142] It is a member of the CsoR/RcnR family

but binds Ni(II) in a four-coordinate planar geometry, as opposed to the octahedral coordination environment in RcnR.[142] Unlike RcnR, InrS does not regulate itself as shown by an Δ*inrS* deletion strain of *Synechocystis,* which showed an increase in the number of *nrsD* transcripts but not *nrsB (*Inrs).[142] InrS is regulated by NrsR, which binds in the *nrsR-inrS* intergenic region and additionally regulates *nrsA.* InrS binds the intergenic region between *nrsC* and *nrsD* at an $ATAC_3$-N_3-G_5TAT consensus sequence. InrS has a K_d for Ni(II) of 2.05 x 10^{-14} M, higher than any other known metal sensor in *Synechocystis*, and can remove Ni(II) from the other sensors directly. Cys53, His78, and Cys82 were confirmed as three out of four of the Ni(II) binding ligands in InrS, with the fourth ligand still unknown.[143] *In vitro*, Co(II), Cu(I) and Zn(II) cause InrS to dissociate from DNA like Ni(II) and this was confirmed *in vivo* for Cu(I) and Zn(II) after metal addition to the media but only at 1 hour.[143] Thus, InrS is promiscuous and can respond to metals other than Ni(II) *in vivo* as long as the metal concentration is high enough. The orthologous NcrB in *Leptospirillum ferriphilum* is also Ni(II) responsive and controls both the exporters *ncrA* and *ncrC,* as well as itself.[144]

1.4.4 FrmR

Formaldehyde is a natural substance present at an estimated concentration of 100 μM in the blood of a healthy human.[145] In bacteria formaldehyde is formed from methylglyoxal, a product of glycolysis, when it reacts with glycine to degrade it.[145,146] Formaldehyde is known to be highly toxic to humans and animals, but also to bacteria, and is widely used as a disinfectant.[147–149] As an electrophile it reacts rapidly with free thiols and amines on proteins and DNA.[150–152] Both of these processes result in substantial crosslinking.[153–155] Because of its toxicity, most organisms, and especially

human pathogens, possess a formaldehyde detoxification system. In *E. coli* and *Synechocystis* the formaldehyde stress response, consisting of FrmA and FrmB, is regulated by FrmR.[156,157] Although part of the CsoR/RcnR family, and most closely homologous to RcnR, FrmR has been shown to bind to a sequence consisting of six G/C base pairs flanked by AT-rich regions, and release DNA to allow for transcription only in response to formaldehyde and not to any metals.[156,157] It is thought to react with formaldehyde through its single cysteine,[109] which is the only residue conserved throughout the entire family. Because of its sequence similarity with RcnR, FrmR was mutated with the intention of generating an RcnR-like metal site which would theoretically impart metal response.[157] FrmRE64H became sensitive to Zn(II) and Co(II) but this was not due to generation of a metal site, as WT FrmR was shown to also be capable of binding these metals and Cu(I).[157] Instead, a slight increase in metal binding affinity coupled with a decrease in DNA binding affinity generated metal responsiveness. In all instances the endogenous metal sensors outcompeted FrmR for these metals but in the case of Zn(II) the higher K_d allows for partial occupancy of FrmRE64H before the native sensor ZntR is saturated.[157] FrmR detection of Co(II) is glutathione dependent, possible related to FrmAs role as a glutathione dependent formaldehyde dehydrogenase.[156,157]

1.4.5 CstR

Staphylococcus aureus (Sau) lacks the ability to utilize sulfate or sulfite as sulfur sources for the production of cysteine.[158] It can, however, utilize sulfide or thiosulfate as sulfur sources instead,[158,159] both of which are produced in mammals.[160,161] All the genes involved in sulfur metabolism in *Sau* are located on a single operon regulated by CstR

(CsoR-like sulfur-transferase repressor). There are two operator sites in the *cstR-cstA* intergenic region, each containing four G/C base pairs flanked by AT-rich regions.[159] CstR regulates four genes, *tauE, cstA, cstB,* and *sqr*. TauE is not required to mitigate the effects of sulfur stress and is not upregulated by the same stimuli as *cstA, cstB,* or *sqr*.[162] It is hypothesized to be a sulfite/sulfonate effluxer.[159] CstA has three domains, with domain one confirmed to have thiosulfate transferase activity.[163] The function of domains two and three remain unknown. CstB is a multifunctional Fe(II)-persulfide dioxygenase.[164] It has persulfide transferase and thiosulfate transferase activity and oxidizes low molecular weight substrates to generate thiosulfate and reduced thiols to avoid sulfite, which is toxic and not a source of utilizable sulfur for *Sau*.[164] SQR is a sulfide:quinone reductase whose role in *Sau* is unknown. CstR has a K_d of 3.7 nM for these operator regions with a binding mode of two tetramers per operator. Replacement of any of the cystosines abolishes DNA binding. CstR was shown to respond to specific sulfur species, which cause crosslinking and abolish DNA binding. CstR responds to sodium sulfite, sodium hydrosulfide, sodium tetrasulfide, and glutathione pesrsulfide.[159,162] CstR reacts with these species by forming di- and tetra-sulfide bridges between Cys31 of one CstR and Cys60' of another CstR.[165] Modification causes abolition of DNA binding. Individual mutation of C31 and Cys60 to alanine revealed that oxidation begins with Cys31, which is sufficient to reduce DNA affinity by 60 fold as measured by fluorescence anisotropy, and forms a sulfide bridge with Cys60.[165] Oxidation of Cys60 alone causes no attenuation in DNA-binding affinity. However, this does not correlate to *in vivo* experiments, where mutation of either cysteine leads to significant loss of growth in *Sau*.[162] Despite the genes under the control of CstR being

required to survive sulfur stress, deletion of CstR, and thus continuous upregulation of *cstA*, *cstB*, and *sqr*, also causes cell death.[162] RT-PCR of the genes under control of CstR showed that the genes are upregulated 30 fold 10 minutes after introduction to sulfide stress, but after 30 minutes the mRNA levels have returned to pre-stress levels.[162]

1.4.6 RicR

RicR is a Cu-responsive transcriptional regulator in *Mycobacterium tuberculosis*, the second found in this organism with the first being CsoR.[166] It was shown that these two regulators do not influence or control the regulation of the genes under the other's control.[167] In addition to regulating itself, RicR controls the transcription of five other genes; *ipqS* (a putative lipoprotein), *mymT* (a mycobacterial metallothionein), *socAB* (small open reading frame induced by copper A and B), Rv2963 (a putative permease), and *mmcO* (mycobacterial multicopper oxidase).[167] Except for RicR, all of these genes are found exclusively in pathogenic bacteria. Deletion of these genes causes sensitivity to Cu, but deletion or interruption of *ricR* lead to *M. tuberculosis* hyperresistance and hypervirulence in mice. While the source of the hyperresistance was found to be due to *mymT* and *mmcO*, the source of hypervirulence could not be traced back to a single gene. Every gene is controlled by a similar palindrome TACC-N_5-G/AGGT of which *Mt*RicR but not *Mt*CsoR was confirmed to bind.[166,167]

1.4.7 DmeR

DmeR from *Rhizobium leguminosarum* is 39% identical to *E. coli* RcnR.[168] It has a conserved cysteine that aligns with Cys35 in *Ec*RcnR and three conserved histidines that align with His3, His60, and His64. Structural modeling indicated it has three α-helices, similar to CsoR/RcnR. DmeR was shown to regulate DmeF, a Ni(II) and Co(II)

efflux protein, and together they form one operon. Although the DNA-binding site was not confirmed, an RcnR-like conserved palindromic sequence was found upstream of *dmeR* (ATA-X_2-ATA-C_6-TAT-X_2-TAT). Deletion of these genes from the *R. leguminosarum* lead to a decreased tolerance for Ni(II) and Co(II) but no other metals.[168] Transcriptional assays showed that only Ni(II) and Co(II) strongly induced the dmeRF operon, and regulation of the operon occurs upstream of *dmeR* and not between *dmeR* and *dmeF,* which are transcribed as a single unit. While these genes were required for survival under Ni(II) and Co(II) stress for *R. leguminosarum* alone, they have limited or no effects when *R. leguminosarum* is introduced into the roots of lentil and pea plants.[168]

1.4.8 NcrB

NcrB is a nickel responsive metalloregulator in *Leptospirillum ferriphilum.*[144] It has not been tested for any other metals *in vitro* or *in vivo,* but is sequentially most similar to InrS, indicating that Ni(II) may be the only metal it responds to *in vivo*. It has a CsoR-like Cu(I) binding C-H-C motif similar to InrS, with a histidine residue in the fourth position (aligned with His3 in RcnR and His21 in InrS). It binds to a pseudo palindrome, AT-C_5-T-G_7-AT, one upstream of NcrA and one upstream of NcrBC. NcrA and NcrC encode two membrane proteins that form an efflux system.[144]

1.5 Overview

The focus of this dissertation is to identify and understand the function of the ligands that compose the octahedral metal center of the *E. coli* Ni(II)- and Co(II)-responsive transcriptional regulator, RcnR. RcnR is one of the founding members of the CsoR/RcnR family of transcriptional regulators. *In vitro,* RcnR binds a variety of metals,

but *in vivo* studies reveal that RcnR responds only to Ni(II) and Co(II).[72] The ligands bound to the cognate metals exclusively transmit the metal binding event to the rest of the protein, facilitating DNA release and the transcription of the exporter proteins RcnA and RcnB. To study the metal binding ligands, their identity must first be known. However, there is no crystal structure obtained to date and, therefore, homology modeling was performed to gain information on possible metal-binding residues. Various mutations have been made and the functional, structural, and biophysical effects have been assessed using β-galactosidase activity assays, X-ray absorption spectroscopy (XAS), fluorescence anisotropy, and temperature melts.

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CHAPTER 2

GLUTAMATE 34: IS IT A LIGAND, AND WHAT IS ITS ROLE?

2.1 Introduction

As discussed in Section 1.4.2, RcnR is the metalloregulator for the Ni(II) and Co(II) exporter proteins, RcnAB, in *E. coli*. *RcnR (Resistance to Cobalt and Nickel Repressor)* is also a founding member of the recently discovered CsoR-RcnR family of transcriptional regulators. RcnR is responsive to both Ni(II) and Co(II). RcnR responds to binding of these metals by releasing the promoter region of the *rcn* operon, allowing for transcription. Studies on CsoR, a Cu(I) responsive transcriptional regulator, indicates that DNA release is caused by a small conformational change that disfavors DNA binding.[1] However, the dissimilarities among CsoRs, and this family of regulators in general, does not rule out other mechanisms.

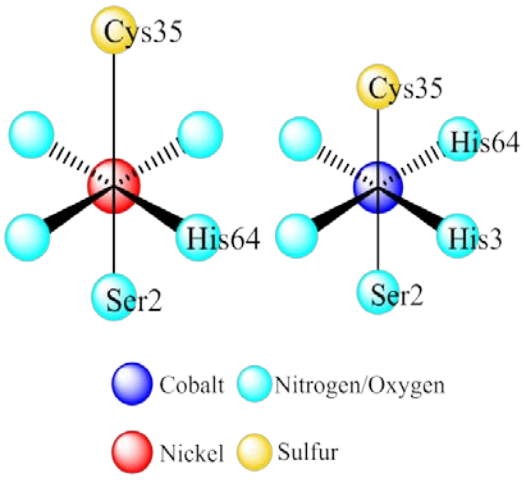

Figure 2.1: Representation of the metal site structure of Co(II) and Ni(II), with known metal binding residues identified.

RcnR binds both cognate metals in an octahedral geometry, with Ni(II) binding the N-terminus, Cys35, and His64 (**Figure 2.1**). This leaves three coordination positions

whose ligand identities are unknown. XAS suggests that all three of them are N/O-donor ligands and at least one of them is a histidine. RcnR binds Co(II) utilizing the N-terminus, His3, Cys35, and His64 (**Figure 2.1**). This leaves two coordination positions of unknown identity although XAS suggests that both are N/O-donor ligands and neither is histidine. The two cognate metals are not necessarily expected to utilize the same residues to complete the coordination spheres. Existing data already suggests different ligands are used, (Co(II) binds His3 and Ni(II) does not).[2] In order to understand how RcnR is selecting its cognate metals to the exclusion of other metals, it is necessary to study the first coordination sphere because this is most likely to have the greatest effect on metal response.

Analysis of the amino acid sequence of RcnR reveals that ~25% of the amino acids are potential metal binding residues. In order to narrow down the focus of the investigation, homology modeling using the Modeller v9.12[3] was performed by Dr. Francesco Musiani and Dr. Stephano Ciurli at the University of Bologna. The model of tetrameric apo-*Ec*RcnR was previously determined and is based upon an average of all available crystal structures of CsoR, a copper-dependent transcription factor within the RcnR family.[3] The same procedure, crystal structures, and sequence alignments were used to model the metal-bound forms of *Ec*RcnR using Modeller v9.12. Constraints were taken from published information regarding the Ni(II) and Co(II) site structures available from prior XAS analyses to guide the calculations.[4] The best fitting model provides the lowest value of the Modeller DOPE score.[5] In the best fitting models, both Ni(II) and Co(II) coordinated a glutamate in the primary coordination sphere. However, for each

metal the glutamate is a different residue. For Ni(II) the glutamate ligand is Glu34 and for Co(II) the glutamate is Glu63.

The goal of this investigation is to experimentally identify the remaining residues bound to Ni(II) and Co(II) and determine whether Glu34 is a Ni(II) ligand and contribution to RcnRs function as a metalloregulator. The design uses a point mutation strategy where Glu34 is mutated to Ala, losing a putative ligand, and to Cys, resulting in a putative ligand substitution. Structural effects of these mutations on the metal site were assessed by X-ray absorption spectroscopy (XAS), giving information on coordination number, ligand type, and metal-ligand bond distance. *In vivo* mutation functional effects were assessed using transcriptional reporter assays that monitor β-galactosidase activity. Transcriptional responses at low metal ion concentrations were determined using β-galactosidase assays in tandem with metal titrations. Size-exclusion chromatography (SEC) was used to determine quaternary structure of the mutants.

2.2 Experimental Procedures

2.2.1 RcnR Mutagenesis

Point mutations for producing E34A-, E34C-RcnR protein variants were introduced into the wild-type RcnR gene on a pET22-b vector using the QuikChange (Stratagene) site-directed mutagenesis method. The mutations for E34A-RcnR and E34C-RcnR were made using the primers ATGCTCGACGAGCCGCACGCATGCGCTGCAGTTTTAC and ATGCTCGACGAGCCGCACTGTTGCGCTGCAGTTTTAC and their reverse complements, respectively. NovaBlue (Novagen) competent cells were transformed with

the PCR product and mutant plasmids were isolated from transformants on a plate containing ampicillin. The presence of the desired mutation was confirmed in each case via sequencing at GENEWIZ Inc. (South Plainfield, NJ).

2.2.2 RcnR Expression and Purification

Plasmids encoding WT-RcnR and its variants were used to transform DL41 (DE3) pLysS cells for protein expression. A single colony of *E. coli* DL41 (DE3) pLysS with the plasmid encoding an RcnR protein was grown overnight at 37 °C in a Luria-Bertani broth (LB) culture supplemented with ampicillin (amp) at 100μg/mL and chloramphenicol (cam) at 34μg/mL. An aliquot (20 mL) of the overnight culture was added to 2 L of fresh LB with amp (100μg/mL) and cam (34μg/mL) added. The cultures were incubated at 37 °C with shaking until an OD_{600} of ~0.8 was reached and then induced by addition of β-D-1-thiogalactopyranoside (IPTG) (CarboSynth) to a final concentration of 0.8 mM. The temperature was dropped to 20 °C and the cultures were incubated overnight for 10-12 hours. Centrifugation separated harvested cells, suspended in residual media, and frozen at -80 °C. The lysed cells were thawed in a 37 °C water bath, and each liter of culture was treated with 20 μL DNase I solution (10mg/mL DNase I, 40% glycerol), 45 μL of 1 M tris(2-carboxyethyl)-phosphine hydrochloride (TCEP) (Soltech Ventures), and 65 μL of 200 mM phenylmethyl-sulfonylfluoride (PMSF) (MP Biomedicals). The lysed cells were then incubated at 37 °C for 45 minutes.

Chromatographic purification of RcnR employed an AKTA-FPLC system (Amersham Biosciences) and a peristaltic pump (Gilson). The soluble cell fraction from 1 L of cell culture was loaded onto a 5 mL HiTrap Heparin HP column (GE Life Sciences) equilibrated with 20 mM Hepes, 1 mM TCEP, 5 mM EDTA, 10% glycerol,

300 mM NaCl at pH 7.0 (buffer A). The protein was washed with buffer A and then eluted in one step using 30% buffer B (20 mM Hepes, 1 mM TCEP, 5 mM EDTA, 10% glycerol, 1 M NaCl at pH 7.0). The protein was eluted in four 5 mL fractions and the fraction containing RcnR (as determined by SDS-PAGE) was then split into two 2.5 mL fractions and loaded on a 120 mL HiLoad 16/60 Superdex 75 (GE Life Sciences) column equilibrated with buffer A. Fractions were collected on the basis of absorbance at 280 nm. An SDS-PAGE gel was run to determine which fractions contained RcnR. The fractions containing RcnR were diluted to 200 mM NaCl and loaded onto a hand packed 5 mL SP Sepharose HP column. The column was washed with buffer C (20 mM Hepes, 1 mM TCEP, 5 mM EDTA, 10% glycerol, 50 mM NaCl at pH 7.0) and then the protein was eluted in a single step using 40% buffer B and 60% buffer C in three fractions, collecting 4.5 mL in the first fraction and 5 mL in the next two. The purity of the fractions was checked using SDS-PAGE. Fractions containing RcnR were estimated to be >90% pure and were used without further purification. The expected molecular weights of the purified proteins were confirmed using electrospray ionization mass spectrometry (ESI-MS) using an ABI-SCIEX QSTAR-XL equipped with a turbo-spray ESI source and a Agilent 1100 HPLC system with a BioBasic-8 (Thermo Scientific) column for salt removal. Alternatively, samples were measured by direct injection following exchange into 200mM ammonium acetate using a Zeba desalting column. The molecular weights of WT-, E34A-, E34C-RcnR isolated proteins were: calc'd: 10002.7 Da, found: 10002.6 Da; calc'd: 9944.7 Da, found: 9945.0 Da; calc'd: 9976.7 Da, found: 9975.9.

2.2.3 Metal Complexes of RcnR Proteins

All proteins, except where noted, were concentrated to ~150 μM and buffer

exchanged twice using a buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP, 10% glycerol at pH 7.0 (buffer M). The exchange used 10 mL Zeba spin desalting columns (Thermo Scientific) with a 7k molecular weight cutoff to remove EDTA and exchange the NaCl for NaBr. In the case of the two samples in NaCl (Co(II) and Ni(II) E63A), samples were prepared using the same procedure except instead of NaBr, the buffer contained 300 mM NaCl. XAS experiments used NaBr to distinguish cysteine S-donors from Cl^- ligands for EXAFS analysis, and to identify solvent accessible coordination sites.

Protein concentrations were confirmed using the experimentally determined extinction coefficient ε_{276} of 2530 M^{-1} cm^{-1} on samples denatured with 8 M guanidine hydrochloride.[6] Four aliquots of a 50 mM stock solution in water providing 2.5 equivalents of $Ni(OAc)_2$ or $Co(OAc)_2$ (Fisher Scientific), or 1.5 equivalents of $Zn(OAc)_2$ were added to the apo-RcnR solutions to produce the respective RcnR complexes. The protein samples equilibrated overnight with the added metal ions before incubation with Chelex (Sigma Aldrich) beads for ~30 minutes removing nonspecifically bound metal ions. The protein solutions analysis for metal content used an ICP-OES with a Perkin-Elmer Optima DV4300 ICP-OES instrument. This analysis was performed by preparing RcnR samples with an expected metal concentration of 1 ppm using the previously determined protein concentrations. The metal: protein (monomer) ratios for samples prepared in buffer M were as follows: WT-RcnR, 1.2:1 for Ni(II), 0.8:1 for Co(II), 0.7:1 for Zn(II); E34A-RcnR, 0.4:1 for Ni(II), 0.6:1 for Co(II), 0.5:1 for Zn(II); E34C-RcnR, 0.2:1 for Ni(II), 1:1 for Co(II), 0.7:1 for Zn(II).

2.2.4 X-ray Absorption Spectroscopy (XAS)

Samples of the metallated proteins were concentrated to ~1-4 mM of metallated protein and a total volume of ~50 μL in buffer M (unless otherwise noted) using microspin concentrators (Millipore). The concentrated samples were injected into polycarbonate XAS sample holders wrapped in kapton tape. The XAS sample holders were rapidly frozen in liquid nitrogen and stored at -80 ^{o}C.

XAS data collections for the Ni(II) complexes of WT-, E34A-, and E34C-RcnR as well as the Zn(II) complexes of E34C-RcnR were done on beam line X3B at the National Synchrotron Light Source (NSLS), Brookhaven National Laboratories (Upton, NY). For data collected at NSLS, the samples were cooled to ~50 K using a He displex crysostat, and under ring conditions of 2.8 GeV and 120-300 mA using a sagittally focusing Si(111) double-crystal monochromater. X-ray fluorescence was collected using a 30-element Ge detector (Canberra). Z-1 filter between the sample chamber and the detector minimized any scattering.

Data for the Co (II) complexes of WT-, E34A-, and E34C-RcnR and Zn (II) WT-, and E34A-RcnR complexes were collected at the Stanford Synchrotron Radiation Laboratory (SSRL) on beam line 7-3. For data collected at SSRL, the samples were cooled to ~10 K using a liquid helium cryostat (Oxford Instruments) . The ring conditions were 3 GeV and 450-500 mA. Beam line optics included an Si(220) double-crystal monochromator. X-ray fluorescence data was collected using a 30 element detector (Canberra) at beam line 7-3. Soller slits with a Z-1 element filter was placed between the sample chamber and the detector to minimize scattering. Internal energy calibration was performed by collecting spectra simultaneously in transmission mode on the corresponding metal foil to determine the first inflection point on the edge, which was set

to 7709.5 eV for Co, 8331.6 eV for Ni, or 9660.7 eV for Zn. X-ray absorption near-edge structure (XANES) data were collected from -200 to +200 eV relative to the metal K-edge. Extended X-ray absorption fine structure (EXAFS) data were collected to 15*k* above the reference edge energy.

2.2.5 Data Reduction and Analysis

The SixPack software[7] program was used to remove bad channels, average the data and to perform energy calibrations, in addition to data reduction and normalization. Edge normalization and background subtraction were performed using a Gaussian pre-edge function and a seven section, fourth-order polynomial spline between k = 2 Å^{-1} and k = 14 Å^{-1} for the post-edge region, followed by normalization of the edge jump.

The Artemis software program was used to provide EXAFS analysis based on the EXAFS equation with parameters generated using FEFF6.[8,9] The EXAFS equation is:

$$\chi(k) = \sum_i \frac{N_i f_i(k) e^{-2k^2\sigma_i^2}}{kr_i^2} \sin[\,2kr_i + \delta_i(k)]$$

where *f(k)* is the scattering amplitude, *δ(k)* is the phase-shift, *N* is the number of neighboring atoms, *r* is the distance to the neighboring atoms, and σ^2 is the disorder to the nearest neighbor. The data were converted to *k*-space using the relationship: $k = [\frac{2m_e(E-E_0)}{\hbar^2}]^{1/2}$. The k^3-weighted data were Fourier-transformed over a *k*-range of 2-12.5 Å^{-1} using a Kaisser-Bessel window for all data sets, and fit in *r*-space using an S_0 value of 0.9. All *r*-space spectra shown are not phase-corrected. Shells of S- or N- scattering atoms and imidazole rings were fit with separate values Δr_{eff} ($r - r_{eff}$) or the change in metal-ligand bond distance with respect to the input path distance and σ^2 with initial values of 0.0 Å and 0.003 Å^2, respectively. Each fit was initiated by setting a universal E_0

(7723 eV for Co, 8340 eV for Ni, and 9670 eV for Zn) and an initial ΔE_0 of 0 eV, which was allowed to vary for each fit. The multiple-scattering contributions from histidine imidazole ligands fits were over an *r*-space range of 1-4 Å.

Histidine ligands were fit as geometrically rigid rings with a variable angle, α, with α defined as the rotation around an axis perpendicular to the plane of the ring through the coordinated nitrogen. The distances of the five non-hydrogen atoms in the imidazole ring were fit in terms of a Δr_{eff} for various angles (α = 0 – 10°).[10–12] Multiple-scattering parameters for imidazole ligands bound to nickel, cobalt and zinc were generated using the FEFF6 software package with the initial input based on average bond lengths and angles gathered from crystallographic data.[12,13] All paths with amplitude contribution ranks larger than 16 were included.[4]

To assess the goodness of fit from different fitting models, the fit parameters χ^2, reduced χ^2 ($r\,\chi^2$), and R-factor were minimized. Increasing the number of adjustable parameters is generally expected to improve the R-factor; however χ^2 may go through a minimum, the increase indicating that the model is overfitting the data. Parameters are:

$$\chi^2 = \frac{N_{\text{idp}}}{N_{\varepsilon^2}} \sum_{N}^{i=1} \{\text{Re}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2 + \text{Im}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2\}$$

And

$$r\chi^2 = \frac{\chi^2}{N_{\text{idp}} - N_{\text{var}}}$$

Where N_{idp} is the number of independent data points, $N_{\text{idp}} = \frac{(2\Delta r \Delta k)}{\pi}$, Δr, is the fitting range in *r*-space, where Δk is the fitting range in *k*-space. Here N_{ε^2} is the number of uncertainties to minimize, Re () is the real part of the EXAFS Fourier-transformed data and theory functions, Im () is the imaginary part of the EXAFS Fourier-transformed data

and theory functions, and $\tilde{\chi}(R_i)$ is the Fourier-transformed data or theoretical function.

The calculated R-factor for each fit is proportional to χ^2 and represents the root-mean-square difference between the data and calculated fit. This is expressed by:

$$\boldsymbol{R} = \frac{\sum_{i=1}^{n}\{\mathrm{Re}[\tilde{\chi}_{data}(R_i) - \tilde{\chi}_{theory}(R_i)]^2 + \mathrm{Im}[\tilde{\chi}_{data}(R_i) - \tilde{\chi}_{theory}(R_i)]^2\}}{\sum_{i=0}^{n}\{\mathrm{Re}[\tilde{\chi}_{data}(R_i)]^2 + \mathrm{Im}[\tilde{\chi}_{data}(R_i)]^2\}}$$

2.2.6 β-Galactosidase Transcription Reporter Assays

Starter cultures of *E. coli* strain PC113 (Δ*rcnR*) cells containing WT or mutant *rcnR* genes on the *rcnR-PrcnA-lacZ* plasmid (pJI114)[14] were grown aerobically overnight at 37 °C in Luria-Bertani broth (LB) with chloramphenicol. These cultures were used to inoculate duplicate cultures in 2.0 mL LB with chloramphenicol in sterile culture tubes. These cultures were grown to an OD_{600} ~0.3-0.7 and then placed on ice to arrest cell growth. The OD_{600} of each culture was recorded prior to placing 200 µL of culture into a 2.0 mL micro-centrifuge tube containing 800 µL of the β-galactosidase buffer (60 mM Na_2HPO_4, 40 mM NaH_2PO_4, 10 mM KCl, 1 mM $MgSO_4$, and 50 mM β-mercaptoethanol), 20 µL 0.1% SDS and 40 µL chloroform. The tubes were then vortexed for 5 seconds and incubated at 28 °C for 10 minutes. A solution of 200 µL of *o*-nitrophenyl-β-galactosidase (ONPG) (4 mg/mL) was added to each tube and the time recorded. The tubes were inverted 2-3 times and incubated at 28 °C. Upon completion of the inversion, the reaction was quenched by adding 1M Na_2CO_3 and the time recorded. Transcription activity was calculated in Miller Units using the equation $U = \frac{(1000)A_{420}}{(t)(v_{cells})(OD_{600})}$ where A_{420} is the absorbance at 420 nm, t = time of the reaction in minutes, v_{cells} is the volume of cells added to the reaction, and OD_{600} is the recorded OD taken after placing cells on ice.

Metal induction experiment cells were treated using the same technique except that before addition of cells to the duplicate cultures, a maximal concentration of metal resulting in < 10% inhibition of growth was added to each culture. This corresponded to: 300 μM $Zn(OAc)_2$, 130 μM $CoCl_2$, and 700 μM $NiCl_2$ for each metal sample in Figure 2.5. All measurements were performed in quadruplicate. A one-way ANOVA followed by Dunnett's test for multiple comparisons determined statistical significance.

Metal titration experiments were performed using the identical technique used for metal induction experiments. Metal was added to each individual culture with a range of 0 – 180 μM $CoCl_2$ and 0 – 900 μM $NiCl_2$. All measurements were performed in quadruplicate.

Data for all experiments is shown in Tables A.3-A.10.

2.2.7 Circular Dichroism

Far-ultraviolet CD spectra were carried out on a Jasco J-1500 CD spectrometer. Wavelength scans (20 nm/min, 2 nm step size) were performed on 20 μM apo-WT-RcnR protein and the variants, and 20 μM metal-substituted WT-RcnR protein and the variants in buffer (10 mM Hepes, 150 mM NaCl, 5% glycerol at pH 7.0) that was allowed to equilibrate with 1 equivalents of metal for 4 h. Each spectrum was the accumulation of four scans, and the background buffer scans were subtracted from each.

2.2.8 Size Exclusion Chromatography

Size-exclusion chromatography was performed using a Superdex 75 15/300 GL (GE Healthcare) column. The column was standardized using albumin (66 kDa), carbonic anhydrase (29 kDa), cytochrome c (12.4 kDa), and aprotinin (6.5 kDa). A standard curve was constructed by plotting V_e/V_0 versus the molecular mass (where V_e is the elution

volume of the peak, and V_0 is the elution volume of thyroglobulin), and the data were fit with a second order polynomial. All proteins were injected onto the column at a concentration of 500 μM (monomer) in 20 mM HEPES, 150 mM NaCl, 5 mM EDTA, 1mM TCEP, 10% glycerol, pH 8.0, and the retention volumes of the peak(s) (V_e/V_0) from each chromatogram were analyzed using the standard curve to determine the molecular weights of the eluted proteins.

2.3 Results

2.3.1 X-ray Absorption Near Edge Spectroscopy (XANES) Analysis of E34A- and E34C-RcnR

X-ray absorption spectroscopy (XAS) was used to examine the metal site structures of complexes of WT-RcnR and RcnR Glu34 variants to determine if Glu34 is a first coordination sphere ligand and involved in distinguishing cognate (*i.e.,* Co(II) and Ni(II)) from noncognate (*e.g.,* Zn(II)) metals.

Determination of coordination number and geometry of a metal center used X-ray absorption near-edge structure (XANES) analysis. Metal ions, such as Co(II) and Ni(II), that have vacancies in the 3d orbitals exhibit features below the edge energy that involve 1s→3d electronic transitions. This transition is symmetry-forbidden in centrosymmetric geometries, and intensities of these features (peak areas) provide a measure of the centrosymmetricity of the metal site. Peak areas are smaller for more centrosymmetric geometries, such as octahedral and square-planar, and larger for noncentrosymmetric geometries, such as tetrahedral and square pyramidal.[15,16] Geometries lacking one or more axial ligands (planar or pyramidal) have a peak associated with a 1s→4p_z electronic

transition that is observed and can be used to differentiate between centrosymmetric

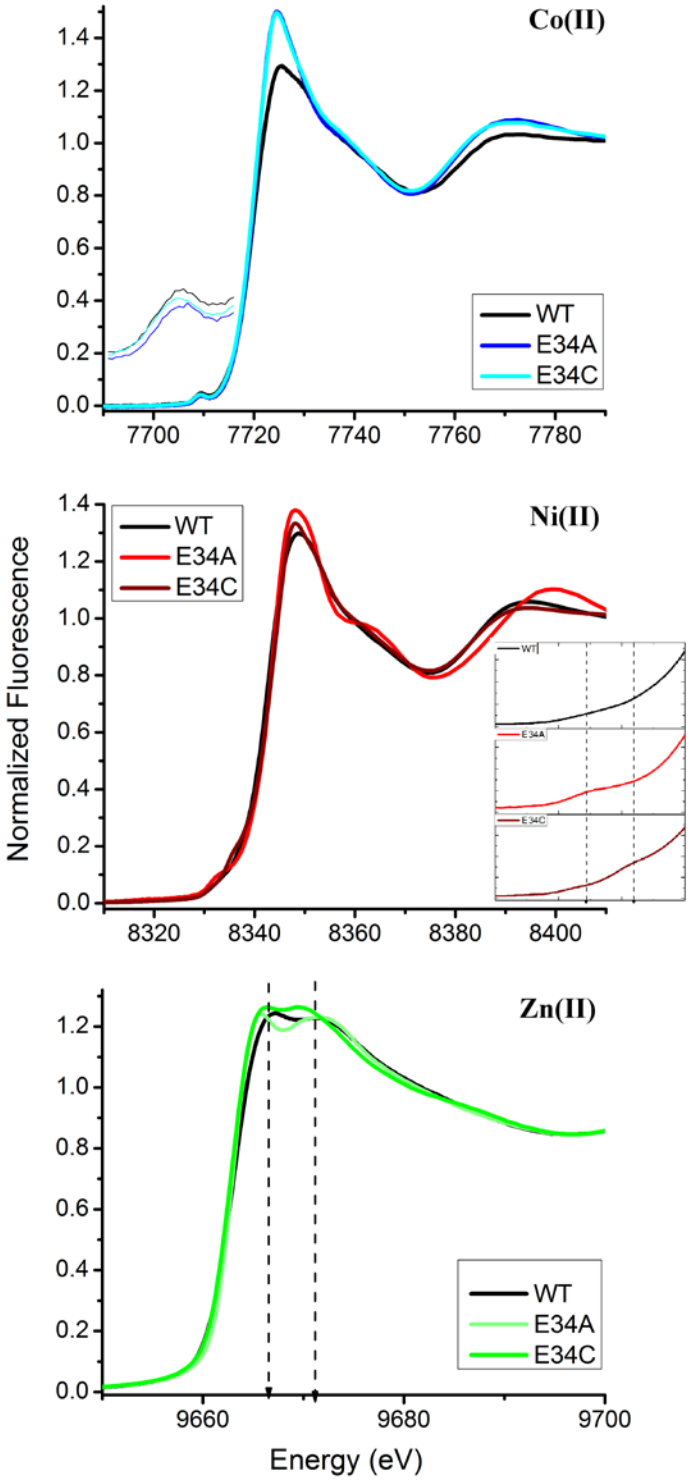

Figure 2.2: *K*-edge XAS spectra of WT-, E34A-, and E34C-RcnR with cognate metals Co(II) (Top), Ni(II) (Middle), and Zn(II) (Bottom) in buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP and 10% glycerol at pH 7.0.

geometries, *e.g.*, square-planar and octahedral, and between five-coordinate pyramidal and trigonal bipyramidal complexes.[16] Being a d^{10} metal, Zn(II) lacks vacancies in the 3d manifold, and no 1s→3d transition is possible. However, the number and intensity of transitions near the white line is strongly affected by coordination number and ligand type, allowing a qualitative analysis of the XANES spectra to be made for Zn(II).[17,18] XANES data for WT-RcnR and the Glu34 variants is summarized in **Table 2.1** and **Figure 2.2**.

Co(II) complexes. A single pre-edge feature at ~7710 eV that is associated with a 1s→3d transition (**Figure 2.2**) is observed for the Co(II) complexes of both E34A- and E34C-RcnR proteins. The relatively small peak areas (**Table 2.1**) indicate the Co(II) centers have centrosymmetric ligand arrangements.[16,19] The small peak areas coupled with the lack of other pre-edge features, is consistent with an octahedral geometry. This finding indicates no change in geometry associated with the mutation of Glu34 compared to WT-RcnR.[20,21] However, the XANES spectra for WT-, E34A- and E34C-RcnR are non-overlapping, indicating some change to the Co(II) coordination sphere. EXAFS analysis examines these differences.

Ni(II) complexes. The pre-edge features of the Ni(II) complexes of E34A- and E34C-RcnR proteins are very different and distinct from the six-coordinate Ni(II) WT-RcnR complex. Both Glu34 variants exhibit a peak associated with a 1s→3d transition located at ~8330 eV (**Figure 2.2**). The peak area for the E34A-RcnR complex is very large (~ 10 x 10^{-2} $Å^2$), indicating a non-centrosymmetric geometry. While a tetrahedral geometry is possible, it is inconsistent with XANES analysis, which supports a seven-coordinate fit. The peak area for the Ni(II) E34C-RcnR complex is ~ 5 x 10^{-2} $Å^2$, which

coupled with a shoulder associated with a 1s→4p_z transition at ~8336 eV, is most consistent with a five-coordinate pyramidal complex.[19,20,22]

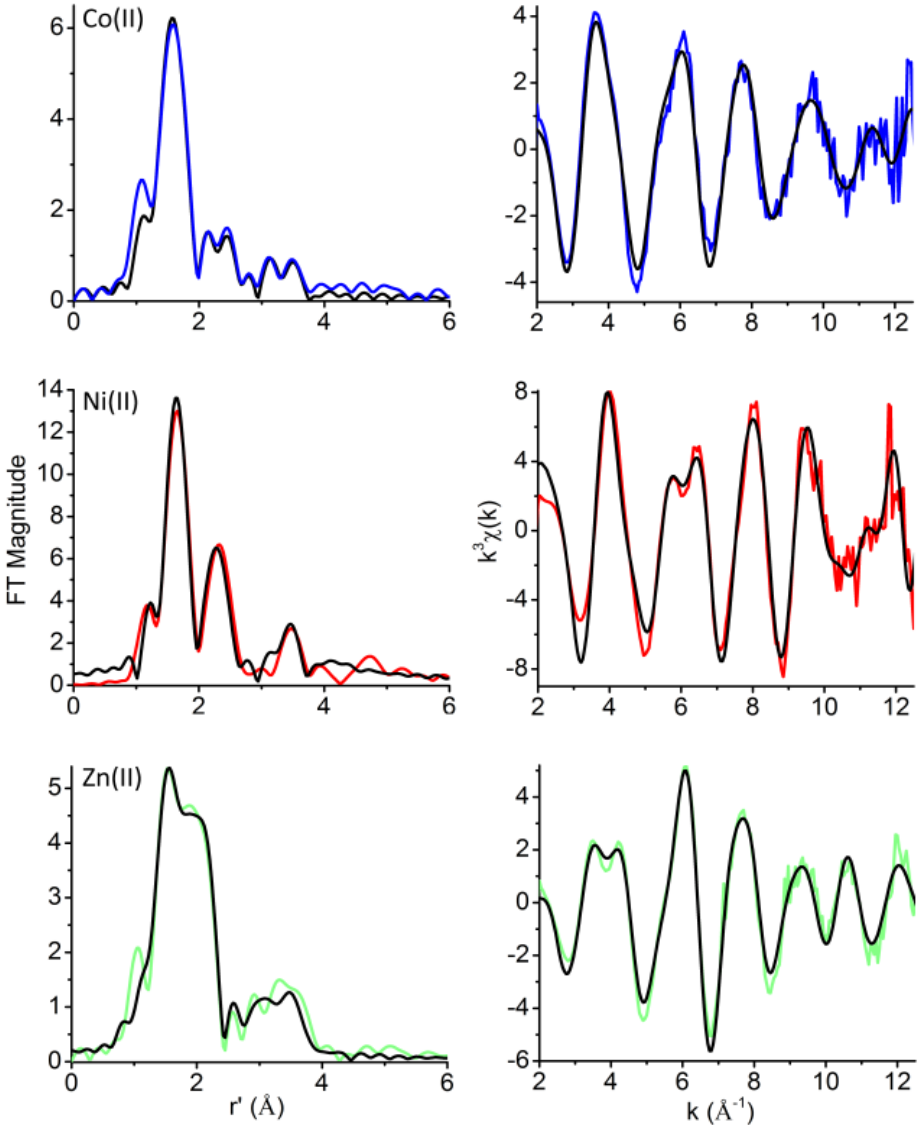

Figure 2.3: K-Edge XAS spectra of E34A-RcnR metal complexes in buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP and 10% glycerol at pH 7.0: (Left) Fourier-transformed EXAFS data (colored lines) and fits (black lines). (Right) Unfiltered k^3-weighted EXAFS spectra and fits.

The XANES analysis can be interpreted as a mixture of four-coordinate planar and six-coordinate complexes averaging out to a five-coordinate complex. This interpretation may explain the small 1s→3d transition observed for Ni(II) E34C-RcnR,

since the mixture contains only centro-symmetric Ni(II) sites. Regardless of the interpretation, a significant change has occurred in the Ni(II) site structure.

Zn(II) complexes. The normalized intensities of the post edge XANES features for the Zn(II) complexes of E34A- and E34C-RcnR are ~1.3. These features indicate four- or five-coordinate Zn(II) sites.[17] XANES spectra of both Zn(II) complexes (**Figure 2.2**) exhibit features at 9666.6 and 9671.0 eV associated with 1s→4p transitions, consistent with a Zn(II) center coordinated by a combination of N/O-donors and ligands with heavier scattering donor-atoms; such as sulfur or bromide.[18]

2.3.2 Extended X-ray Absorption Fine Structure (EXAFS) Analysis of E34A- and E34C-RcnR

Extended x-ray absorption fine structure (EXAFS) analysis was used to provide metal-ligand distances with an accuracy of ~ ±0.02 Å. Combined with information on scattering atoms (Z ± 2), and a second estimate on the coordination number (± ~20% total number of ligands), the analysis is complementary to the XANES analysis. The EXAFS spectra and best fits are summarized in **Figure 2.3** and **Figure 2.4** and **Table 2.1**. Comprehensive fitting tables are included in **Appendices E** and **F**. XAS data for WT-RcnR samples were rerun and data fit using Artemis allowing for a direct comparison between WT-RcnR and the variants.

Co(II) complexes. EXAFS analysis of Co(II) E34A-RcnR (**Table 2.1, Figure 2.3**) is consistent with a six-coordinate site, agreeing with the XANES analysis. The best fit consists of two histidine imidazole ligands, two N/O-donors, a bromide from buffer and a sulfur-donor that indicates coordination of Cys35. Incorporation of the Br^- ligand supports an open coordination site, or solvent-exchangeable ligand, in the E34A-RcnR

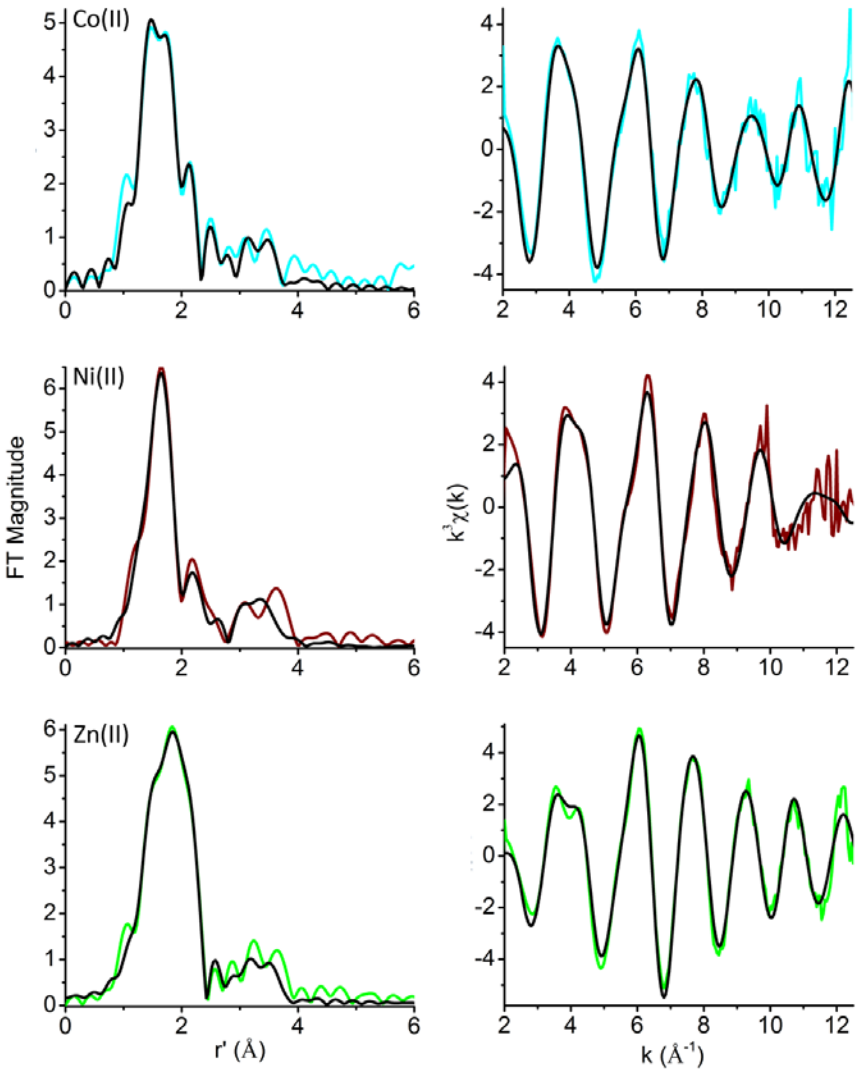

Figure 2.4: K-Edge XAS spectra of E34C-RcnR metal complexes in buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP and 10% glycerol at pH 7.0: (Left) Fourier-transformed EXAFS data (colored lines) and fits (black lines). (Right) Unfiltered k^3-weighted EXAFS spectra and fits.

complex that does not exist in WT-RcnR. The replacement of an N/O donor ligand with a Br- suggests that loss of a first-coordination sphere ligand has occurred. The E34A-RcnR site has a long Co-S bond at 2.54(4) Å that is significantly altered from the Co-S distance in the Co(II) WT-RcnR complex (2.20 Å), and more closely resembles the WT-RcnR Ni(II)-SCys35 bond distance (2.63 Å). The $(His)_2(N/O)_2(SCys)Br$ ligand is consistent with Glu34 as a Co(II) ligand in WT-RcnR.

Table 2.1: XANES and EXAFS Analysis for Metal Complexes of E63A-, E63C-RcnR Mutant Proteins in Buffer with 300 mM NaBr.

	XANES Analysis				EXAFS Analysis				
Sample	K-edge energy (eV)	$1s \rightarrow 3d$ peak area ($x10^2$ eV)	$1s \rightarrow 4p_z$ observed	Coord #/geometry	Shell	*r* (Å)	σ^2 ($x10^{-3}$ Å^2)	ΔE_0 (eV)	%R
				WT-RcnR					
Co(II)	7720.2	6(1)	No	6	1 N/O	1.97(4)	2(3)	-2(2)	4.1
					2 N/O	2.20(4)	0(2)		
					1 S	2.20(6)	5(6)		
					1 Imd 0°	2.09(4)	4(3)		
					1 Imd 10°	2.09(3)	2(3)		
Ni(II)	8342.7	2(1)	No	6	2N/O	2.07(2)	2(2)	4(1)	3.8
					1N/O	2.21(3)	3(4)		
					1S	2.63(2)	6(2)		
					1Im 0°	2.07(3)	3(2)		
					1Im 10°	2.02(6)	6(5)		
Zn(II)	9663.0	NA	NA	5	**1N/O**	**1.94(3)**	**7(4)**	**-4(1)**	**1.2**
					1S	**2.30(2)**	**7(3)**		
					1Br	**2.41(1)**	**5(1)**		
					1Im 0°	**1.99(2)**	**0(3)**		
					1Im 10°	**2.10(2)**	**1(2)**		
				4	1S	2.30(2)	5(2)	-5(1)	1.5
					1Br	2.41(1)	5(1)		
					1Im 0°	2.07(2)	2(1)		
					1Im 0°	1.95(2)	0(2)		
				E34A-RcnR					
Co(II)	7720.6	6(1)	No	6	1N/O	2.02(1)	5(1)	2(2)	1.7
					1N/O	2.16(1)	6(1)		
					1S	2.54(4)	1(4)		
					1Br	2.50(3)	3(3)		
					1Im 0°	2.02(7)	6(9)		
					1Im 0°	2.16(8)	6(11)		
Ni(II)	8343.9	10(1)	No	6	1N/O	2.04(1)	13(1)	7(1)	3.2
					2N/O	2.19(2)	9(2)		
					1S	2.60(2)	3(2)		
					1Im 0°	1.94(2)	9(1)		
					1Im 0°	2.10(2)	3(2)		
				7	**2N/O**	**2.07(1)**	**9(1)**	**7(1)**	**3.2**
					2N/O	**2.22(2)**	**7(2)**		
					1S	**2.61(1)**	**3(1)**		
					1Im 0°	**1.94(2)**	**8(1)**		
					1Im 0°	**2.11(2)**	**7(1)**		
Zn(II)	9663.0	NA	NA	5	**1N/O**	**1.98(4)**	**7(6)**	**-3(1)**	**1.9**
					1S	**2.28(3)**	**9(4)**		
					1Br	**2.43(1)**	**6(1)**		
					1Im 0°	**2.11(2)**	**2(2)**		
					1Im 0°	**1.98(2)**	**1(2)**		
				4	1S	2.27(3)	8(3)	-4(2)	2.9
					1Br	2.42(1)	6(1)		
					1Imd	1.96(1)	2(1)		
					1Imd	2.09(2)	2(2)		
				E34C-RcnR					
Co(II)	7720.4	6(1)	No	6	1N/O	1.99(3)	1(3)	3(2)	1.5
					1N/O	2.14(2)	4(2)		
					1S	2.36(4)	7(4)		
					1S	2.61(4)	8(4)		
					1Im 0°	2.17(4)	1(3)		
					1Im 0°	2.01(3)	1(2)		

Ni(II)	8344.3	5(2)	Yes	5	1N/O 1S 1S 1Im 0° 1Im 0°	2.04(2) 2.29(2) 2.56(3) 1.94(3) 2.08(3)	1(2) 3(2) 9(3) 2(3) 1(2)	1(2)	2.5
Zn(II)	9662.9	NA	NA	5	**1N/O** **1S** **1Br** **1Im** **1Im**	**2.02(3)** **2.29(1)** **2.41(1)** **1.99(3)** **2.11(4)**	**6(5)** **3(2)** **7(1)** **3(5)** **3(5)**	**-2(1)**	**1.1**

The EXAFS data from Co(II) E34C-RcnR is consistent with a six-coordinate complex and the XANES analysis (**Table 2.1, Figure 2.4**). The major change in the structure with respect to Co(II) WT-RcnR is the inclusion of two S-donor ligands (Cys34 and Cys35), one at a long distance (2.61(4) Å) and one at a shorter distance (2.36(4) Å). The data are best fit by a model including two His imidazole ligands, with a split N/O shell, where the difference in the M-N/O distances between the two shells (0.15 Å) is at the calculated resolution of the data set ($r = \frac{\pi}{2\times\Delta k} = 0.15$). Although it is not possible to identify which Cys residue is responsible for the long vs. short Co-S distances, the $(His)_2(N/O)_2(SCys)_2$ ligand set for the E34C-RcnR Co(II) site also supports the assignment of Glu34 as a Co(II) ligand in Co(II) WT-RcnR.

Ni(II) complexes. The analysis of the EXAFS spectrum of the Ni(II) E34A-RcnR complex is best fit with a ligand environment composed of two histidine imidazole ligands, four additional N/O-donor ligands in two resolved shells, plus a long (~2.61(1) Å) Cys35 S-donor, totaling seven scattering atoms (**Table 2.1 and Figure 2.3**). Although a six-coordinate complex would be within the coordination number error determination by EXAFS analysis (±20%), a centrosymmetric arrangement of ligands (four-coordinate planar and octahedral) is inconsistent with the large 1s→3d transition observed in the XANES spectrum. Seven-coordinate geometry is most consistent with both the EXAFS and XANES analyses, although a distorted six-coordinate complex can't

be excluded. The %R of an identical six-coordinate fit is indistinguishable from a seven-coordinate (**Table 2.1)**, but a high σ^2 for one nitrogen shell is unlikely. The E34A-RcnR Ni(II) site is essentially unaltered from Ni(II) WT-RcnR (**Table 2.1**). The complex does not bind exogenous Br^-, as expected for a 'loss of ligand' variant, consistent with Glu34 not being a ligand in Ni(II) WT-RcnR. However, a complex involving replacement of Glu34 by a water molecule in preference to Br^- cannot be ruled out. The substitution of Glu34 by water, however, would change the charge on the metal center and would be inconsistent with the incorporation of Br^- in Co(II) E34A-RcnR.

In contrast to the Ni(II) E34A-RcnR complex, the EXAFS data from Ni(II) E34C-RcnR indicates a decrease in the coordination number from six to five (**Table 2.1, Figure 2.4**). This change in coordination is consistent with the XANES result, which indicated a five-coordinate pyramidal geometry. The EXAFS analysis also reveals that the Ni(II) center in E34C-RcnR has two S-donor ligands (Cys34 and Cys35), with one long WT-like Ni-S distance at 2.56(3) Å, and a shorter Ni-S bond at 2.29(2) Å. This finding is consistent with the XANES five coordinate pyramidal geometry. Neither the E34A- nor the E34C-RcnR Ni(II) sites give the expected results for the 'loss of ligand' or 'ligand substitution' variations, in contrast to the corresponding Co(II) complexes.

Zn(II) complexes. The EXAFS data analysis of Zn(II) complexes of E34A- and E34C-RcnR (**Table 2.1, Figure 2.3 and 2.4**) are consistent with the qualitative XANES analysis. The EXFS analysis indicates Zn(II) sites in these variants are essentially identical, and very similar to Zn(II) WT-RcnR. The best fits in all cases include two His ligands, one N/O-donor ligand, one Br^- ligand and one S-donor. The resulting five-coordinate $Zn[His_2(N/O)(SCys)Br]$ complexes are also empirically indistinguishable

from the Zn(II) WT-RcnR complex, demonstrating Glu34 is not a ligand for Zn(II) in WT-RcnR.

2.3.3 β-Galactosidase Activity Assays

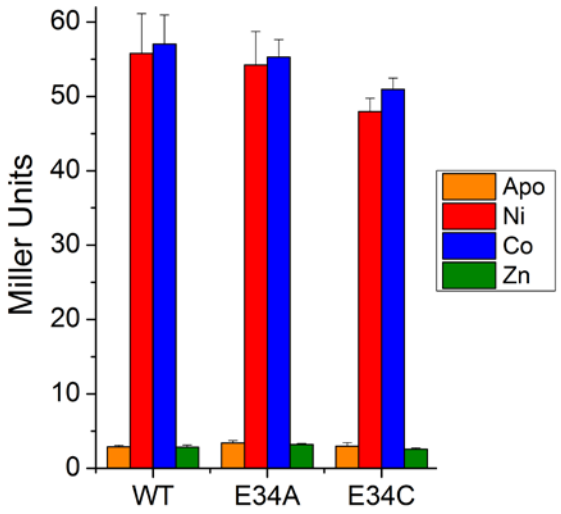

Figure 2.5: β-galactosidase assay showing the effect of the E34A-, and E34C-RcnR mutations on the expression of *PrcnA* in response to binding metal ions. The data is an average of four replicates. The error bars represent standard deviation.

A β-galactosidase reporter assay (**Figure 2.5**) tested the Glu → Ala and Glu → Cys mutants on RcnR metal responsiveness. Previous studies[6] revealed that expression of P_{rcnA} is induced only in the presence of Ni(II) and Co(II), and not induced with addition of Mn(II), Fe(II), Cu(II), Zn(II), and Cd(II). Both E34A- and E34C-RcnR had indistinguishable metal ion responses from WT-RcnR; demonstrating ligation of Glu34 is not important to metal-induced transcription, regardless of the structural role. Both Glu34 variants remain unresponsive to Zn(II) binding, indicating metal selectivity is not impaired by Glu34 alterations. These results indicate that while Glu34 mutation affects metal site structure, it does not affect the transcriptional regulation function of RcnR.

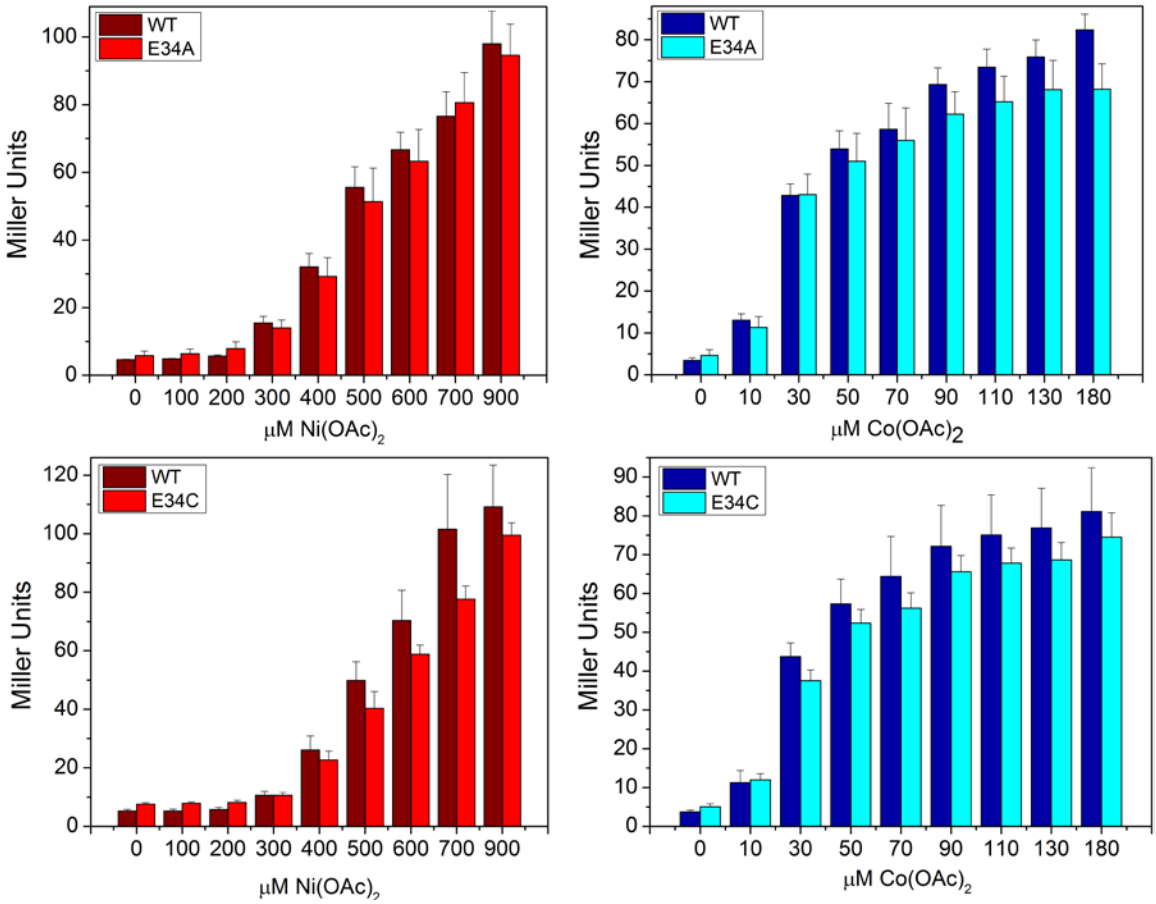

Figure 2.6: β-galactosidase reporter assay titrations showing the effect of the E34A-, and E34C-RcnR mutations on the expression of *PrcnA* in response to binding metal ions. The data is an average of four replicates. The error bars represent standard deviation.

The β-galactosidase assays **(Fig.2.6)** were performed at metal concentrations producing maximal activity without detriment to cell growth. Although the Glu34 mutations showed no difference at maximal metal concentrations, metal titrations were examined to determine if variations affected the β-galactosidase activity. There was no difference between WT-RcnR and the response of Glu34 variants at concentrations ranging from 0 μM to 900 μM (**Figure 2.6**). Interestingly, WT-RcnR begins to respond to both Ni(II) and Co(II) at very different metal concentrations, with response beginning at ~300 - 400 μM $NiCl_2$ and ~10 μM $CoCl_2$.

2.3.4 Circular Dichroism (CD) and Size Exclusion Chromatography (SEC)

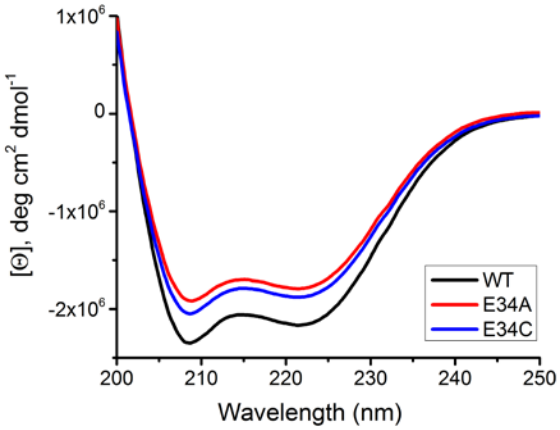

Figure 2.7: CD spectra of apo WT-, E34A-, and E34C-RcnR proteins in 20 mM HEPES, 100 mM NaCl, 1 mM TCEP, 5% glycerol, pH 7.0.

Changes to RcnR's secondary structure with variants of Glu34 were assessed using circular dichroism. In all cases the spectra are dominated by features at 208 nm and 222 nm corresponding to α-helices and is in line with previous research (**Figure 3.8**).[6] This finding does not rule out possible changes in secondary structure. The addition of Co(II) or Ni(II) yielded no obvious change in the CD spectrum of the variants as compared to additions made in WT-RcnR (**Appendix A, Figure A.2**). There was no observed change in quaternary structure by size exclusion chromatography (**Figure 3.9** and **Table 3.3**), as all proteins were found to be tetrameric.

Table 2.2: Theoretical and experimentally derived molecular weights as determined by SEC.

Sample	Theoretical MW (kDa)	Experimental MW (kDa)	Quaternary Structure
WT-RcnR	40.0	43.7	Tetramer
E34A-RcnR	39.8	40.7	Tetramer
E34C-RcnR	39.9	42.2	Tetramer

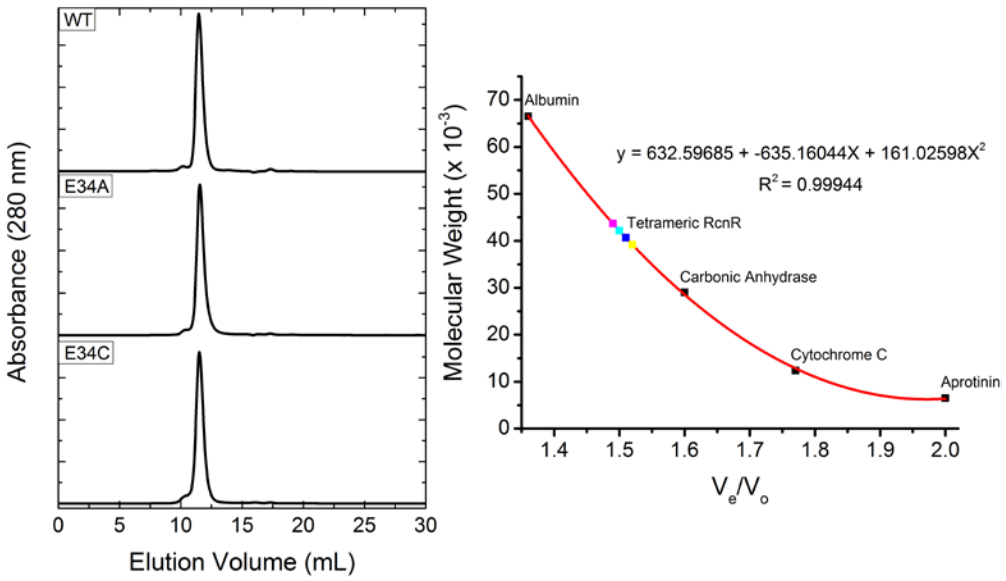

Figure 2.8: (Left) SEC chromatogram of apo WT-, E34A-, and E34C-RcnR proteins in 20 mM HEPES, 150 mM NaCl, 5 mM EDTA,1 mM TCEP, 10 % glycerol, pH 7.0 (Right) Retention volume versus molecular mass for the standards and RcnR proteins. The green dot represents WT-RcnR, the blue dot represents E34A-RcnR, the cyan dot represents E34C-RcnR, the pink dot represents E63A-RcnR and the yellow dot represents E63C-RcnR. The red line represents a second order polynomial fit for the standards.

2.4 Results Summary

The results clearly associate Glu34 with cognate metal binding and demonstrate altering Glu34 to alanine or cysteine causes significant changes to the cognate metal site structures, but not to the non-cognate Zn(II) site structure. These changes do not disrupt allosteric responses to specific metal binding required for DNA release, even at low metal concentrations (**Figure 2.5 and 2.6**). In the case of Co(II) E34A-RcnR, one of the N/O-donor ligands was replaced with a bromide from solvent. A vacant first-coordination position around the Co(II) center is the most likely cause, consistent with the loss of a ligand (Glu34). In the E34C-RcnR mutation, one of the N/O-donor ligands surrounding the Co(II) center was replaced with an S-donor ligand. As there are only two cysteines in the protein, and the buffer consists of Br- ions instead of Cl- ions, the only explanation is the second S-donor ligand comes from Glu34Cys. These two results taken together

indicate that Glu34 is a Co(II) ligand in RcnR.

The nature of the structural changes observed for the Ni(II) complexes are more ambiguous. In the Ni(II) complexes, alteration of Glu34 to alanine is best described as a seven-coordinate complex with an $(N/O)_6S$ ligand donor atom set. One possible explanation is that Glu34 is a Ni(II) ligand, and the vacancy in E34A-RcnR is filled either by a water molecule in preference to bromide, or by causing Glu63 to become bidentate to fill the vacancy. The combination of these two changes would result in a seven-coordinate complex, with Glu63 becoming bidentate to compensate for the increased positive charge on the metal. However, this seems less likely because loss of Glu34 without coordination of an anion would change the net charge on the Ni(II) complex.

A similar situation was observed for Ni(II) H3E-RcnR mutation, which also adopted a 7-coordinate site hypothetically due to a bidentate glutamate binding. Yet, another explanation is that Glu34 is involved in structural ordering of another glutamate (or aspartate) in the first coordination sphere of the Ni(II) center. Upon mutation to alanine, this first coordination sphere ligand is no longer ordered and binds bidentate. This would not disrupt the net charge surrounding the metal center.

In the case of Ni(II) E34C-RcnR, the substitution of Glu34 by cysteine results in multiple structural changes--the loss of a N/O-donor ligand and substitution of another by Cys34 yielding a five-coordinate complex with two S-donor ligands ($(N/O)_3S_2$). This change is not consistent with a simple ligand substitution and therefore obscures the role of Glu34 as a ligand. Although the sequence of these perturbations is not apparent, one plausible explanation is that substitution of Glu34 by cysteine stabilizes a low-spin

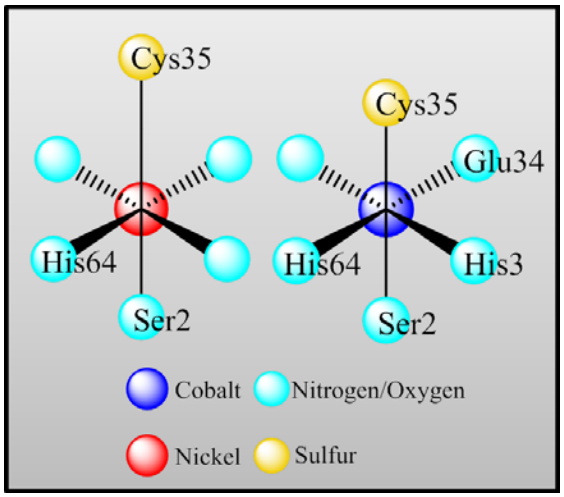

Figure 2.9: New representation of the metal site structure of Co(II) and Ni(II), with known metal binding residues identified.

configuration favoring additional ligand loss. Alternatively, loss of Glu34 could lead to a low-spin configuration, which then coordinates Cys34. Taken together, the analysis is not clear if Glu34 is a Ni(II) ligand. What is clear is that it holds little to no importance in terms of metal selectivity or functional response to metal.

2.5 Discussion

The studies performed on Glu34 highlight a discrepancy in the field of metal responsive transcriptional regulators, and metalloproteins in general. There is no correlation between the first coordination sphere structures of RcnR bound to Ni(II) and Co(II) and function as a transcriptional regulator. In every mutation examined, there is an obvious structural change without functional change nor a change in *in vivo* metal selectivity. These findings are odds with current hypothesis, which maintain coordination sphere ligand type and geometry are critical for function.[23–27] This hypothesis should technically be correct, as metal binding is the signal inducing metalloregulator function. If the structure around the metal center is not important, then the question remains on

what is metal binding doing that imparts function.

The results seen for RcnR are not unusual, and a lack of correlation between structure and function has been seen in a variety of other proteins. In the case of the Mn(II) responsive metalloregulator MntR, it binds two six-coordinate Mn(II) ions. The D8M mutation confers Fe(II) sensitivity and binds only one trigonal bipyramidal Mn (II) ion, yet is still fully Mn(II) responsive.[24] Another instance is seen in the case of SmtB, which binds to both Zn(II) and Co(II) in tetrahedral geometries, yet is not Co(II) responsive. However, it is unclear if this is due to a difference in the type of ligands or second coordination sphere interactions.[28] Certain members, such as ArsR (As and Sb responsive) and CmtR (Cd and Pb responsive), bind cognate metals in a trigonal geometry utilizing 3 Cys residues.[29] Despite identical folds, similar amino acid sequences, and identical geometries and ligand types, they have distinct cognate metals. The similarities demonstrate that geometry and first coordination sphere ligand type are not the prevailing factors dictating metal selectivity.

Previous studies of RcnR also show a clear lack of correlation between structure and function, suggesting the function of RcnR is poorly linked to its first coordination sphere. Previous mutations had WT-like metal centers when bound to Ni(II), but had reduced or abolished metal response as seen in the cases of the H60C-, H67C-, and H3C/L-RcnR variants.[2,30] In the case of Co(II), many mutations (H3C, H3E, H60C, H67C) cause the Co(II) center to adopt a structure similar to the WT-RcnR Ni(II) with a characteristic long M-SCys35 bond, yet have a diminished or abolished response.[2,30] The results for Ni(II) and Co(II) together indicate that having a WT-like metal site is insufficient for DNA release based on XAS structural determination. In contrast to the

above cases displaying WT-like structures with a reduced functional response, the H64C-RcnR mutation causes Co(II) to adopt a six-coordinate structure with 3 N/O donor ligands with two S donors and a bromide from solvent. This is a radical change from the WT-RcnR Co(II) structure, and yet retains ~20% of its activity.[30] Previous studies on H3E, H60C, H64C, and H67C mutants of RcnR reveal a 6-coordinate geometry when bound to Zn(II). Yet no activity is conferred, even in the case of H67C which adopts a similar Ni(II) WT-RcnR structure structure.[2,30] This suggests that coordination number alone is not sufficient to alter metal selectivity.

It is possible an exact replication of coordination number and ligand type is not necessary for RcnR, and possibly other metalloregulators. The lack of correlation between ligation of specific Glu residues and transcriptional response in *E. coli* RcnR indicates not every ligand in the primary coordination sphere plays a critical role in the allosteric response regulating transcription. In this study, variation of Glu34 is unimportant to transcription, while variation of Glu63 results in a partial loss of transcriptional response (Chapter 3). The data suggests specific ligands are critical for function and the loss of these specific ligands disrupts the internal structural rearrangement needed for allosteric switching. The findings indicate WT-RcnR operates via a 'switch' mechanism, where binding of one or two specific residues governs the allosteric rearrangement. This situation is similar to what has been determined for the Ni(II)/Co(II) responsive membrane-bound periplasmic regulator CnrX.[31–34] Mutational studies on CnrX indicate binding of Met123 pulls the protein into a signal propagating active conformation. Non-cognate metals do not bind this residue and thus cannot facilitate this conformational change. The true 'switch' in RcnR appears to be the binding

of the N-terminus, a feature of both cognate metal sites not found for non-cognate metals.[2,30] The switch mechanism can theoretically be extended to His3, as any alteration to either ligand (N-terminus or His3) causes complete functional abolition.

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CHAPTER 3

GLUTAMATE 63: IS IT A LIGAND, AND WHAT IS ITS ROLE?

3.1 Introduction

As mentioned in Section 2.1, this research is focused on the identity of the ligands involved in the first coordination sphere of RcnR. To that end, homology modeling was performed by Dr. Francesco Musiani and Dr. Stephano Ciurli. Their models pointed out that both Ni(II) and Co(II) had a glutamate completing the coordination sphere, but this glutamate was different for each metal. For Ni(II) this glutamate was Glu34 and for Co(II) the glutamate was Glu63.

The goal of the studies in this chapter is to investigate whether Glu63 is a Co(II) ligand and the contribution to RcnRs function as a metalloregulator. This used a strategy employing point mutations of Glu63 to Ala and to Cys, which correspond to "loss of ligand" and "ligand substitution" protein variants (See Chapter 2). The structural effects of these mutations on the metal site will be monitored by X-ray absorption spectroscopy (XAS), providing information on coordination number, ligand type, and metal-ligand bond distance. *In vivo* functional effects of these mutations will be monitored by β-galactosidase transcriptional reporter assays. Changes in DNA binding affinity of the protein variants will be examined via fluorescence anisotropy experiments. The effect on the quaternary structure of RcnR was determined by size-exclusion chromatography (SEC).

3.2 Experimental Procedures

3.2.1 RcnR Mutagenesis

Point mutations for producing E63A-, and E63C-RcnR protein variants were introduced into the wild-type RcnR gene on a pET22-b vector using the QuikChange (Stratagene) site-directed mutagenesis method. The mutation for the E63A-RcnR variant was made using the primers CGGGAAGTGATTAAAGGTCATCTGACGGCACACATC and CATCCCCCTGGTGAACGATGTGTGCCGTCAG. The mutation for the E63C-RcnR variant was made using the primers CGGGAAGTGATTAAAGGTCATCTGACGTGCCACATC and CATCCCCCTGGTGAACGATGTGGCACGTCAG. The PCR product was transformed into NovaBlue (Novagen) competent cells, and mutant plasmids were re-isolated from transformants on an agar plate containing ampicillin. The presence of the desired mutation was confirmed in each case via sequencing at GENEWIZ Inc. (South Plainfield, NJ).

3.2.2 RcnR Expression and Purification

The E63A- and E63C-RcnR proteins were overexpressed and purified (Chapter 2, Section 2.2.2) using single colonies of *E. coli* DL41 (DE3) pLysS with the plasmid encoding the E63A- E63C- mutant proteins. The molecular weights of E63A- and E63C-RcnR proteins are; calc'd: 9944.7 Da, found: 9945.1 Da; calc'd: 9976.7 Da, found: 9976.8 Da, respectively.

3.2.3 Metal Complexes of RcnR

Metal substituted E63A and E63C proteins were prepared in a buffer containing 20 mM Hepes, 300 mM NaBr and 10 % glycerol at pH 7.0 (buffer M) using the method

described in Chapter 2.2.3. NaBr was used in XAS experiments to distinguish cysteine S-donors from Cl^- ligands in the EXAFS analysis, and to identify solvent accessible coordination sites. Metals were added to the protein as outlined in Section 2.2.3 of Chapter 2. Excess and non-specifically bound metals were removed by chelex treatment. Protein concentrations were confirmed using the experimentally determined extinction coefficient ε_{276} of 2530 M^{-1} cm^{-1} from protein denatured with 8 M guanidine hydrochloride.[1] Metal concentrations were determined by taking aliquots of the protein solution that would make a ~1 ppm metal sample when diluted to 1 mL with deionized water. The precise metal content was then determined using a Perkin-Elmer Optima DV4300 ICP-OES instrument. The metal: protein ratios obtained for samples prepared in buffer M with NaBr are as follows; E63A-RcnR, 0.4:1 for Ni(II), 0.3:1 for Co(II), 0.3:1 for Zn(II); E63C-RcnR, 0.5:1 for Ni(II), 0.2:1 for Co(II), 0.6:1 for Zn(II).

3.2.4 X-ray Absorption Spectroscopy (XAS)

Samples of the metallated proteins were concentrated to ~1-4 mM metallated protein and a total volume of ~50 μL in buffer M (unless otherwise noted) using microspin concentrators (Millipore). The concentrated samples were injected into polycarbonate XAS sample holders wrapped in kapton tape, and then rapidly frozen in liquid nitrogen and stored at -80 ^oC. All the samples were run at NSLS or SSRL under the same conditions stated in Chapter 2 Section 2.2.4.

XAS data collections for the Co(II) E63C-RcnR complex, the Ni(II) complexes of E63A- and E63C-RcnR, and the Zn(II) complexes of E63A-, and E63C-RcnR were performed on beam line X3B at the National Synchrotron Light Source (NSLS), Brookhaven National Laboratories (Upton, NY). Beam line 9-3 generated the data for the Co(II) E63A- RcnR complex in NaBr. The Stanford Synchrotron Radiation Laboratory

(SSRL) beam line 7-3 generated the data collected for the Ni(II) and Co(II) complexes of E63A-RcnR in NaCl buffer.

3.2.5 Data Reduction and Analysis

All the data in this chapter were handled as outlined in Chapter 2, Section 2.2.5.

3.2.6 Evans Method

Evans' method NMR experiments were performed on protein samples (2.25 mM Ni WTRcnR and 0.939 mM E34CRcnR) that were buffer exchanged into 20 mM HEPES, 150 mM NaCl, 1 mM TCEP, 5% glycerol, pH 7.0 in 90% H_2O/10% D_2O. 400 µL of protein was placed into an NMR tube and a coaxial insert containing the 10% deuterated buffer was placed inside the NMR tube. Relative shifts between the DSS (4,4-dimethyl-4-silapentane-1-sulfonic acid) reference peak at 0 ppm and the peak shift due to the protein in the outer NMR tube were used to calculate μ_{eff} using equations 1-4:[2,3]

(1) $$\chi_g = \frac{-3\Delta\nu}{4\pi\nu_o m}$$

(2) $$\chi_M = \chi_g M$$

(3) $$\chi'_M = \chi_M - \sum \chi_L$$

(4) $$\mu_{eff} = 2.83\sqrt{\chi'_M T} = \mu_B\sqrt{\vec{L}(\vec{L}+1) + 4\vec{S}(\vec{S}+1)}$$

The equation is expressed where χ_g is the gram susceptibility in cgs units, m is the concentration of metallated protein in g/mL, $\Delta\nu$ is the peak separation in Hz, ν_o is the frequency of the spectrometer in Hz (400.132471 x 10^6 Hz), χ_M is the molar susceptibility, M is the molecular weight of metallated protein in g/mol, χ'_M is the molar susceptibility corrected for protein diamagnetism, χ_L is the diamagnetic shift of the apo-protein, μ_{eff} is the effective magnetic moment in Bohr magnetons, T is the temperature in

Kelvin, $\vec{L}$ is the total angular momentum and $\vec{S}$ is the total spin angular momentum. The diamagnetic correction was determined by comparing the shift of apo versus holo protein at equal concentrations.

3.2.7 β-Galactosidase Reporter Assays

All the data in this chapter were handled as outlined in Chapter 2, Section 2.2.6.

3.2.8 Circular Dichroism

All the data in this chapter were handled as outlined in Chapter 2, Section 2.2.7

3.2.9 Fluorescence Anisotropy

5' TAMRA (5-carboxytetramethylrhodamine) labeled oligonucleotide GATTCTACTCCCCCCCAGTACCTG and non-labeled complementary strand CAGGTACTGGGGGGGAGTAGAATC (*rcnRS1*) were annealed by heating a 10 μM solution of each strand in 10 mM HEPES (pH 7.0) containing 150 mM NaCl, and 5 mM EDTA to 95 °C, and then cooling overnight. WT-, E63A-, and E63C-RcnR were prepared in 10 mM HEPES (pH 7.0) containing 150 mM NaCl, 5 mM EDTA, and 1 mM TCEP (FA buffer). A final DNA concentration of 10 nM was prepared in FA buffer in a 1 cm fluorescence cuvette (Firefly Scientific). RcnR protein was then titrated into the cuvette, and changes in anisotropy were measured using a QuantaMaster-7 2003 fluorimeter (Photon Technology International) fitted with polarizing filters (ex: 543 nm, em: 575 nm, averaging time: 10 s, replicates: 3).

3.3 Results

3.3.1 X-ray Absorption Near Edge Spectroscopy (XANES) Analysis of E63A- and E63C-RcnR

X-ray absorption near-edge structure (XANES) analysis was used to provide information regarding the coordination number and geometry of a metal center. Metal ions, such as Co(II) and Ni(II) that have vacancies in the 3d orbitals, exhibit features below the edge energy that involve 1s→3d electronic transitions. This transition is

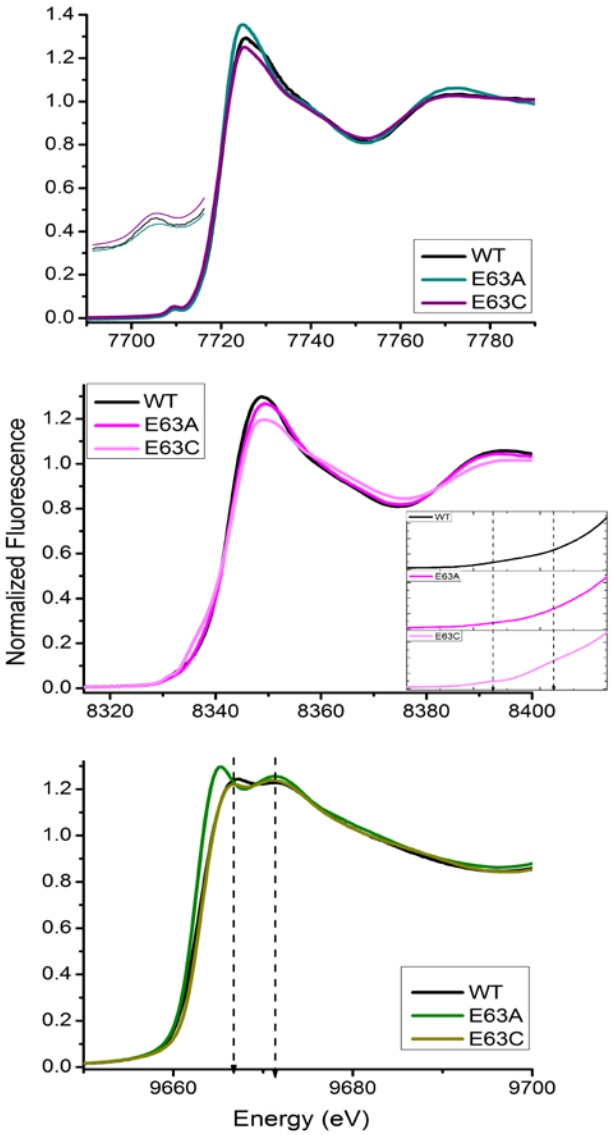

Figure 3.1: *K*-edge XAS spectra of WT-, E63A-, and E63C-RcnR with cognate metals Co(II) (Top), Ni(II) (Middle), and Zn(II) (Bottom) in buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP and 10% glycerol at pH 7.0.

is symmetry-forbidden in centrosymmetric geometries, and the intensities of these features (peak areas) provide a measure of the centrosymmetricity of the metal site. Peak areas are smaller for more centrosymmetric geometries, such as octahedral and square-planar, and larger for noncentrosymmetric geometries, such as tetrahedral and square-pyramidal.[4,5] For geometries lacking one or more axial ligands (planar or pyramidal), a $1s \rightarrow 4p_z$ electronic transition is observed that can be used to distinguish between centrosymmetric geometries, *i.e.*, square-planar and octahedral, and between five-coordinate pyramidal and trigonal bipyramidal complexes.[5] Being a d^{10} metal, Zn(II) lacks vacancies in the 3d manifold and thus no 1s→3d transition is possible. However, the number and intensity of transitions near the white line is strongly affected by coordination number and ligand type, allowing a qualitative analysis of the XANES spectra to be made for Zn(II).[6,7] XANES data for WT-RcnR and the Glu63 variants (**Table 3.1** and **Figure 3.1)**.

Co(II) complexes. The XANES spectra of Co(II) complexes of the E63A- and E63C-RcnR proteins exhibit single pre-edge features at ~7710 eV that are associated with 1s→3d transitions (**Figure 3.1**). The relatively small peak areas found (**Table 3.1**) indicate that the Co(II) centers in these mutants are centrosymmetric.[5,8] The lack of any other pre-edge features is consistent with an octahedral geometry resulting in no change in coordination number or geometry in comparison with Co(II) WT-RcnR, as was the case for the Co(II) E34-RcnR variants.

Table 3.1: XANES and EXAFS Analysis for Metal Complexes of E63A-, E63C-RcnR Mutant Proteins in Buffer with 300 mM NaBr.

	XANES Analysis				EXAFS Analysis				
Sample	K-edge energy (eV)	$1s \rightarrow 3d$ peak area ($x10^2$ eV)	$1s \rightarrow 4p_z$ observed	Coord #/geometry	Shell	*r* (Å)	σ^2 ($x10^{-3}$ Å^2)	ΔE_0 (eV)	%R
				E63A-RcnR					
Co(II)	7720.6	5(1)	No	6	2N/O	2.08(2)	2(2)	-2(1)	2.6
					1S	2.50(2)	4(2)		
					1Br	2.45(2)	1(2)		
					1Im 5°	2.03(3)	4(3)		
					1Im 10°	2.16(6)	7(7)		
Co(II)*	7720.2	6(1)	No	6	1N/O	1.95(5)	5(6)	-2(2)	2.6
					1N/O	2.11(3)	0(3)		
					1S	2.66(5)	8(4)		
					1S (Cl^-)	2.42(4)	8(4)		
					1Im 0°	2.00(2)	2(2)		
					1Im 0°	2.15(2)	2(1)		
Ni(II)	8343.5	>0.5	No	6	2N/O	2.02(2)	3(2)	3(1)	3.5
					1S	2.50(4)	2(4)		
					1Br	2.44(4)	3(4)		
					1Im 0°	2.03(3)	2(3)		
					1Im 10°	2.16(2)	1(2)		
Ni(II)*	8343.1	>0.5	No	6	2N/O	2.01(3)	3(3)	3(2)	3.8
					1S	2.38(5)	9(6)		
					1S (Cl^-)	2.59(3)	5(3)		
					1Im 0°	2.01(8)	9(7)		
					1Im 10°	2.08(5)	3(6)		
Zn(II)	9662.7	NA	NA	5	**1S**	**2.23(2)**	**9(3)**	**-3(1)**	**1.1**
					1Br	**2.40(1)**	**4(1)**		
					1Im 0°	**2.05(1)**	**6(2)**		
					1Im 0°	**2.17(2)**	**2(3)**		
					1Im 0°	**1.93(1)**	**4(1)**		
				4	1S	2.23(2)	9(3)	-5(1)	1.8
					1Br	2.40(1)	4(1)		
					1Imd	2.07(1)	3(1)		
					1Imd	1.94(1)	2(1)		
				E63C-RcnR					
Co(II)	7720.6	7(1)	No	6	2N/O	2.12(3)	9(4)	-3(1)	1.8
					1S	2.28(2)	9(3)		
					1S	2.52(3)	5(2)		
					1Im 0°	2.14(2)	0(2)		
					1Im 0°	1.98(1)	1(1)		
Ni(II)	8342.9	<0.5	Yes	5	1N/O	2.04(2)	1(2)	0(2)	3.7
					1S	2.30(3)	4(3)		
					1S	2.55(4)	8(4)		
					1Im 0°	1.94(4)	2(3)		
					1Im 0°	2.08(4)	2(4)		
Zn(II)	9663.0	NA	NA	5	**1S**	**2.29(3)**	**6(4)**	**-1(2)**	**3.4**
					1Br	**2.40(2)**	**8(3)**		
					1Im 0°	**2.17(3)**	**4(3)**		
					1Im 0°	**2.05(2)**	**7(2)**		
					1Im 0°	**1.93(2)**	**4(2)**		
				4	1N/O	1.96(3)	1(2)	-1(2)	4.4
					1S	2.29(2)	3(2)		
					1Br	2.42(2)	9(3)		
					1Im 0°	2.05(2)	0(1)		

Ni(II) complexes. Neither of the Ni(II) complexes of the E63A- or E63C-RcnR variants have a visible 1s→3d transition, consistent with centrosymmetric Ni(II) environments. Ni(II) E63A-RcnR lacks any other visible pre-edge features, consistent with an octahedral geometry. The E63C-RcnR mutation has a small shoulder that is associated with a 1s→$4p_z$ transition that is not consistent with six-coordinate or trigonal-bipyramidal geometries. The presence of this shoulder is consistent with a five-coordinate pyramidal Ni(II) site, but the small 1s→3d transition is not. This situation could exist if the sample is a mixture of four-coordinate planar and six-coordinate Ni(II) sites, which would exhibit a feature associated with a 1s→$4p_z$ transition from the planar component, but have a small 1s→3d peak area since that is characteristic of both geometries, and average to five ligands in the EXAFS analysis. Regardless of the exact coordination (CN = 5 or 6+4), this variant shows a tendency toward loss of ligands in at least some of the Ni(II) sites, a trend that was also a feature of the Ni(II) E34C-RcnR complex.

Zn(II) complexes. The normalized intensities of the post edge XANES features for the Zn(II) complexes of E63A- and E63C-RcnR are both ~1.3 and indicative of a Zn(II) center with four- or five-coordinate geometry, similar to the Zn(II) sites characterized for WT-, E34A- and E34C-RcnR Zn(II) complexes. The two peaks at ~9666.6 and 9671.0 eV are also observed for Zn(II) E63A-RcnR and Zn(II) E63C-RcnR. The two peaks also indicate a mixed ligand set with N/O- and S-donors, and possibly Br^-.

3.3.2 Extended X-ray Absorption Fine Structure (EXAFS) Analysis of E63A- and E63C-RcnR

Extended x-ray absorption fine structure (EXAFS) analysis was used to provide metal-ligand distances with an accuracy of ~ ±0.02 Å, information on the identity of the

scattering atoms (Z ± 2), and a second estimate on the coordination number (± ~20% total number of ligands) that is complementary to the XANES analysis. The EXAFS spectra and best fits are summarized in **Figure 3.2** and **Figure 3.3** and **Table 3.1**. Comprehensive fitting tables are included in **Appendix G**.

Co(II) complexes. The EXAFS analysis for Co(II) E63A-RcnR spectra also yields similar results to Co(II) E34A-RcnR. The EXAFS analysis is consistent with a six-coordinate geometry, in agreement with the XANES analysis. The best fit includes four N/O donors, two of which are histidine imidazole ligands, one long S-Cys35 donor, and one Br^-, which replaces a N/O-donor ligand in the WT Co site (**Table 3.1** and **Figure 3.2**). The Co-SCys35 distance found (2.50(2) Å) is considerably longer than for the Co(II) WT-RcnR complex, and approaches the distance found in the Ni(II) WT-RcnR complex, as was the case for the Co(II) E34A-RcnR complex. The resulting Co(II)[$(His)_2(N/O)_2$(SCys)Br] complex differs from that found for Co(II) E34A-RcnR only by small differences in Co-L distances. Thus, the data are consistent with Glu63 being a ligand in the Co(II) WT-RcnR complex.

A feature of the best fits of Co(II) E63A-RcnR in NaBr buffer is that the Co-Br distance is shorter than the Co-S distance. An attempt to confirm the assignments was made using buffer containing 300 mM NaCl (**Figure 3.2**), which yields a similar EXAFS fit that is consistent with a Co(II)[$(His)_2(N/O)_2$(SCys)Cl] complex; the major differences being substitution of Br^- by a Cl^- ligand (indistinguishable from and fit as a second S-donor in **Table 3.1**). However, no assignment can be made as the Co-S distances in the Cl^- complex are shorter (2.42 Å) and longer (2.66 Å) than the putative Co-Br^- and Co-S distances. Regardless, the results are consistent with Glu63 being a Co(II) ligand.

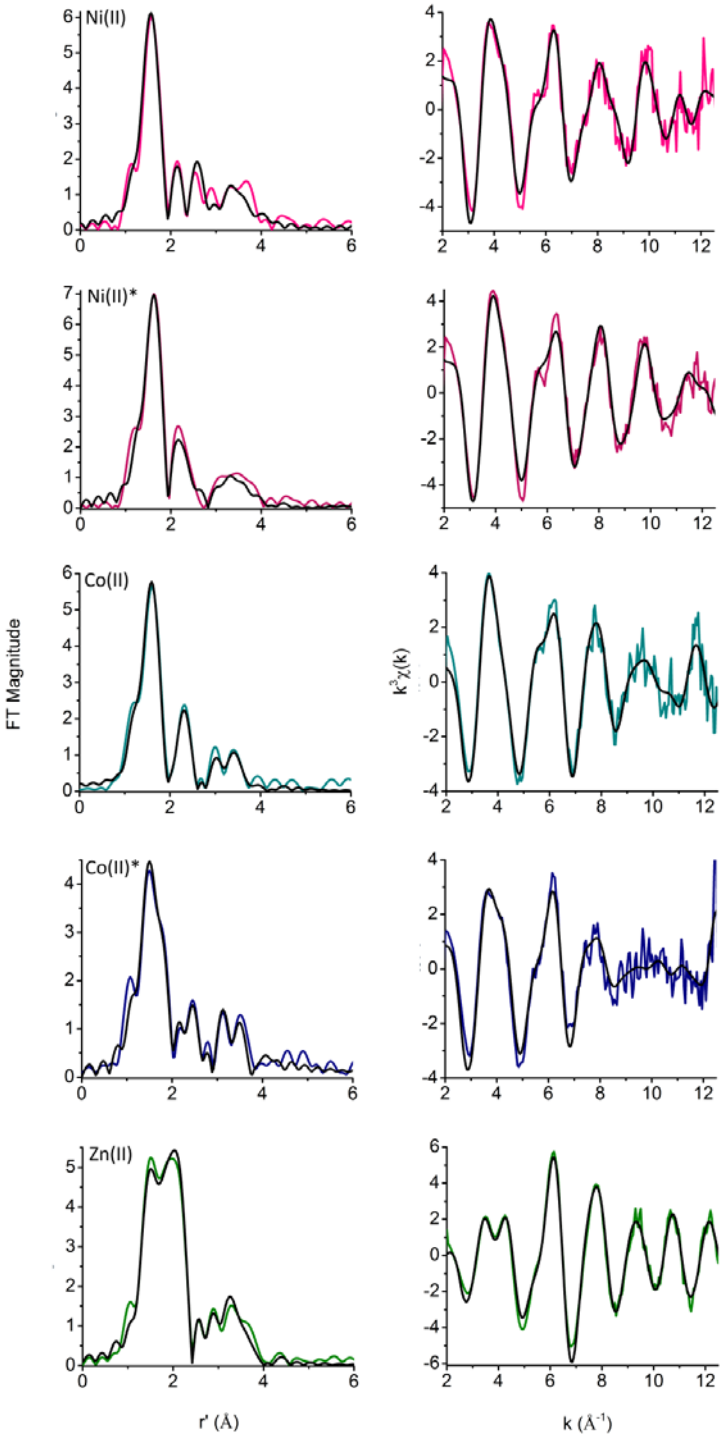

Figure 3.2: K-Edge XAS spectra of E63A-RcnR metal complexes in buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP and 10% glycerol at pH 7.0: (Left) Fourier-transformed EXAFS data (colored lines) and fits (black lines). (Right) Unfiltered k^3-weighted EXAFS spectra and fits.

The results of EXAFS analysis for the Co(II) E63C-RcnR complex (**Table 3.1, Figure 3.3**) also resembles those obtained for the corresponding E34C-RcnR complex, and is also consistent with the formation of a $Co(II)[(His)_2(N/O)_2(SCys)_2]$ complex with

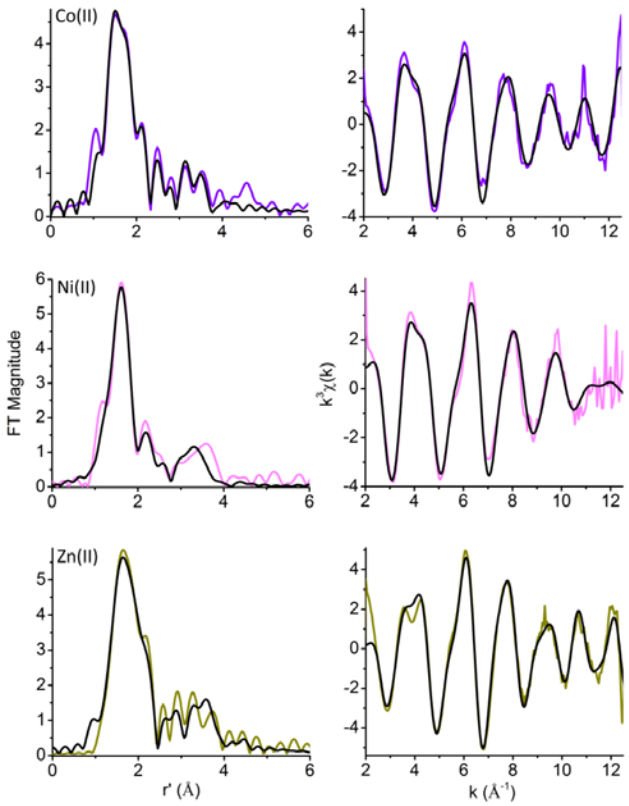

Figure 3.3: K-Edge XAS spectra of E63C-RcnR metal complexes in buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP and 10% glycerol at pH 7.0: (Left) Fourier-transformed EXAFS data (colored lines) and fits (black lines). (Right) Unfiltered k^3-weighted EXAFS spectra and fits.

similar metric parameters. Thus, the results from both variants confirm the role of E63 as a Co(II) ligand in WT-RcnR.

Ni(II) complexes. The EXAFS data for the Ni(II) E63A-RcnR site is best fit by a six-coordinate model that features four N/O-donors, two of which are imidazole ligands (**Tables 3.1**, and **Figure 3.2**). The coordination sphere is completed by a Ni-SCys35 bond (2.50(2) Å) that is shorter than in Ni(II) WT-RcnR (2.63(2) Å), and a bromide ion from

the buffer. This Ni(II)[$(His)_2(N/O)_2$(SCys35)Br] complex results from replacement of Glu63 in Ni(II) WT-RcnR by Br^-, similar to what is observed in the Co(II) complex of E63A-RcnR, and is consistent with Glu63 being a ligand to Ni(II), as well as to Co(II), in the WT-RcnR complexes.

The E63C-RcnR Ni(II) EXAFS spectrum is consistent with a reduced coordination number as compared to WT, changing from six- to five-coordinate. This reduced coordination is similar to observed for E34C-RcnR. Two N/O-donor ligands were lost, one of which was replaced by the Cys63 S-donor, resulting in one long S-donor at 2.55(4) Å and one short at 2.30(3) Å. The large number of structural changes makes it difficult to unambiguously determine which S donor belongs to which cysteine. Taken together, the results of both Glu63 variants are clearly consistent with Glu63 being a Ni(II) ligand in WT-RcnR.

Zn(II) complexes. The EXAFS analysis of Zn(II) E63A-RcnR is indicative of a site composed of three N/O-donors, one S-donor from Cys35 and a bromide from the buffer (**Table 3.1**), and is consistent with expectations based on the XANES analysis (*vide supra*). However, unlike Zn(II) WT-RcnR, where EXAFS data can be modeled as a Zn[$(His)_2$(N/O)(Cys35)Br] complex (**Table 3.1**), the best model for Zn(II) sites in E63A- and E63C-RcnR contains three histidine imidazole ligands, Zn[$(His)_3$(Cys35)Br] (**Table 3.1**, **Figure 3.2** and **3.3**). A WT-like fit for the E63A-RcnR Zn(II) site with two imidazole ligands and 1 N/O ligand, gives slightly lower values of %R and $r\chi^2$ values, but the value of σ^2 for the Zn-SCys35 bond becomes very large, although the Zn-S distance is unchanged between the two models (**Table 3.1**). A similar fit can be obtained for E63C-RcnR, containing two imidazole ligands and 1 N/O-donor ligand, but in this case the fit

gives higher values of %R and $r\chi^2$. The Zn(II) sites in E63A- and E63C-RcnR show subtle structural changes (increased imidazole ligation) that are not consistent with Glu63 being a ligand in the WT-RcnR Zn(II) complex, but suggest an important role for Glu63 in ordering the ligands in Zn(II) site.

3.3.3 Evans Method

It has been seen for the Ni(II) complexes of E34C- and E63C-RcnR that a coordination change has occurred, from octahedral to square-pyramidal. However, a square-pyramidal geometry is inconsistent with the small 1s→3d and leads to the question of why a coordinate change has occurred with a ligand substitution mutation. In a loss of ligand mutation like E34A-RcnR bound to Ni(II), a change in coordination could occur due to substitution by a nearby glutamate. If these glutamate residues are first coordination sphere ligands, a substitution mutation should result in a ligand substitution and not in both a substitution and loss of an additional ligand for two separate mutations

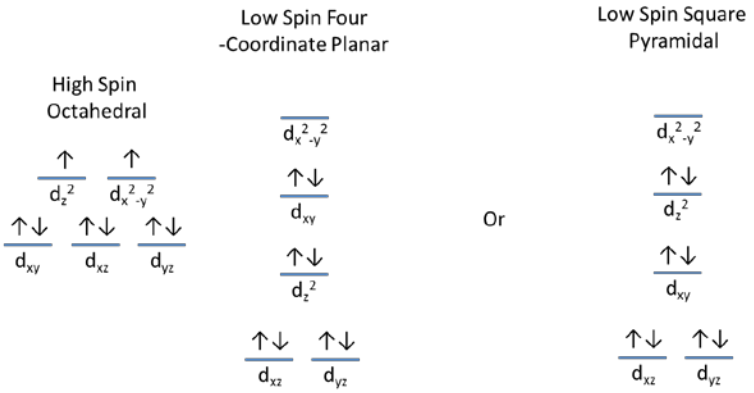

Figure 3.4: Diagram of electron configuration of the d-orbitals in a d^8 complex.

(E34C- and E63C-RcnR). The fact that an identical change has occurred for both glutamate to cysteine mutations but the alanine mutations lead to different coordination

changes must mean that a similar phenomenon is occurring for both the cysteine mutations that may not be due them being first coordination sphere ligands.

The change from octahedral in WT to a square pyramidal geometry in both Cys variants may be due to a spin state change caused by the increased covalency introduced by ligation of the second cysteine ligand. As an octahedral Ni(II) complex is invariably high-spin, a change in spin state to a low-spin complex would necessitate a coordination change. However, the nature of this coordination change is unclear.

Although the 1s→3d transition is small, a square-pyramidal geometry is still supported by XANES. The XANES spectrum is also consistent with a mixture of four-coordinate planar and octahedral geometries. This mixture of geometries would have a small 1s→3d, since it consists of two centrosymmetric geometries, and a 1s→$4p_z$ transition. This is what is observed in the XANES spectrum. In an attempt to distinguish between a low-spin square pyramidal geometry from a mixture of planar and six-coordinate, Evans method was done to test the magnetic susceptibility of the mutant complex as compared with WT-RcnR. A diamagnetic low-spin square pyramidal d^8 complex (**Figure 3.4**) would produce no paramagnetic shift and be distinguishable from a mixture of a diamagnetic S = 0 four-coordinate planar complex and a paramagnetic S = 1 octahedral complex which would result in a magnetic moment less than that of WT-RcnR but greater than a diamagnetic complex.

The WT-RcnR spectrum (**Figure 3.5** and **Table 3.2**) had a peak shifted upfield of the DSS reference peak at 0 ppm. This peak was not present in the buffer spectrum or the apo WT-RcnR spectrum and is attributed to a shift caused by the paramagnetic nickel center. This shift corresponds to the presence of a protein with a μ_{eff} of 3.4 Bohr

magnetons. This is within the expected range (2.8 – 4.0 Bohr Magnetons) for octahedral nickel complexes and indicates a contribution from orbital angular momentum in addition to the spin only value.[9] The E63C-RcnR Ni(II) complex has a small shift upfield of the DSS reference peak which is not present in the spectrum for buffer or the apo-protein, and is attributed to a paramagnetic complex. The difference in Hz between this shift and the DSS reference peak at 0 ppm was used to calculate μ_{eff} for this complex which was 1.54 Bohr magnetons. The presence of a paramagnetic species clearly indicates that this is not a homogenous low-spin square pyramidal complex.

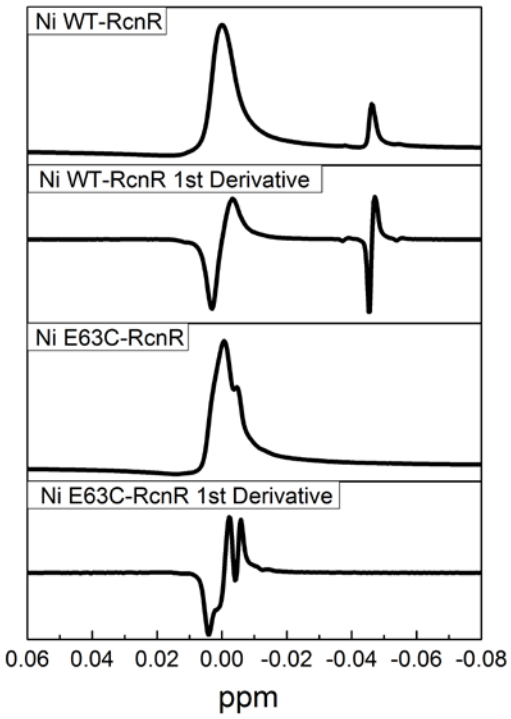

Figure 3.5: 1H NMR spectra of the DSS reference peak in solution with the Ni(II) complexes of WT- and E63C- RcnR in 20 mM HEPES, 100 mM NaCl, 1 mM TCEP, 10% glycerol, pH 7.0 in 90% H_2O/10% D_2O.

Assuming the simplest scenario in which both species in the mixture are present in equal amounts, there are two possibilities that may account for the data. In one possibility, this is caused by the aforementioned mixture of four-coordinate planar and

octahedral geometries. [10–12] A four-coordinate planar complex would have a diamagnetic shift while an octahedral complex would be paramagnetic (**Figure 3.4**) and this mixture would give a value less than that of WT but greater than that of a purely diamagnetic complex, which is what is seen in **Figure 3.5**. Another possibility is a pyramidal complex with a high ⇌ low spin equilibrium,[12–17] in which the energy barrier that typically dictates the spin state of a complex is high enough to prevent a fully high spin complex but low enough to prevent a fully low spin complex (**Figure 3.6**). This mixture would result in a μ_{eff} less than that of WT-RcnR but greater than a purely diamagnetic complex, which is what is seen in **Figure 3.5**.

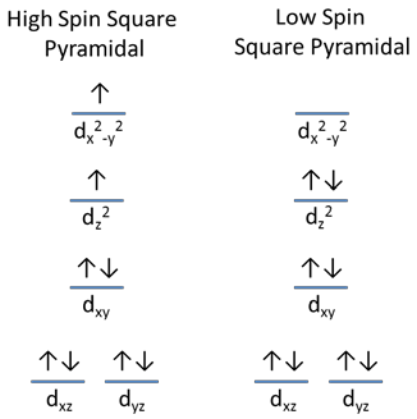

Figure 3.6: Diagram of electron configuration of the d-orbitals in a d^8 square-pyramidal complex.

Table 3.2: Variables used in magnetic susceptibility calculations.

	WT-RcnR	**E63C-RcnR**
Δν	-18.4005 Hz	-1.56944 Hz
ν_0	400.132471 x 10^6 Hz	400.132471 x 10^6 Hz
m	0.0226 g/mL	0.00942 g/mL
M	10061.4 g/mol	10035.4 g/mol
χ_L	4.48 x 10^{-6} cm^3/mol	4.48 x 10^{-6} cm^3/mol
T	298.15 K	298.15 K

Both of these mixtures could result in the observed XANES spectra. There is a third possibility, in which some of the nickel is bound to the protein in a diamagnetic site and some is present in solution as a paramagnetic species. However, this possibility was discarded, as sample preparation involved chelexing, concentration, and buffer exchanging which would remove any unbound metal.

Both of the aforementioned possibilities consist of mixtures, indicating that only a fraction of the sample is responsible for the paramagnetic signal. Assuming that a fully paramagnetic E63C-RcnR species would have a μ_{eff} of 3.4 Bohr magnetons, a back calculation was performed and indicated that ~20% of the sample is paramagnetic. Because XAS is an experiment that average's the structure of all the species in solution the geometries must be approximately equal to each other in order to get a five-coordinate geometry from a mixture of four and six. However, if the mixture is ~20% octahedral then the remaining 80% would be four-coordinate planar and the resulting XANES spectrum would be that of a four-coordinate planar geometry and not five coordinate. This would indicate that E34C- and E63C-RcnR have five-coordinate geometries in a high $\rightleftharpoons$ low spin equilibrium. However, an ~80% diamagnetic sample leads to a third possibility. In this possibility, the diamagnetic species is a low-spin five-coordinate complex and the paramagnetic species is a high-spin octahedral complex. This possibility explains the results of both the Evans method experiment as well as the XANES, which is five-coordinate but with an unusually small 1s→3d due to contributions from the octahedral species. A five-coordinate high $\rightleftharpoons$ low spin equilibrium does not explain the small 1s→3d transition. The data thus indicates that ~80% of E34C-

and E63C-RcnR has lost a ligand upon mutation, with the other 20% retaining six ligands.

3.3.4 β-Galactosidase Activity Assays

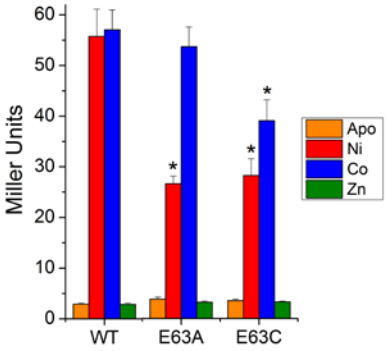

Figure 3.7: β-Galactosidase reporter assay showing the effect of the E63A-, and E63C-RcnR mutations on the expression of *PrcnA* in response to binding metal ions. The data is an average of four replicates. The error bars represents standard deviation and the stars represent statistical significance.

The effect of the Glu → Ala and Glu → Cys mutants on the metal responsiveness of RcnR was tested using a β-galactosidase transcription reporter assay (**Figure 3.7**). Previous studies[1] revealed that expression of P_{rcnA} is induced only in the presence of Ni(II) and Co(II), with no induction upon the addition of Mn(II), Fe(II), Cu(II), Zn(II), and Cd(II). The E63A-RcnR variant also shows a WT-like response to Co(II), but its activity is reduced by ~50% in response to Ni(II). The E63C-RcnR variant also shows a ~50% reduction in response to Ni(II), but also has a perturbed Co(II) response, being ~75% of the WT-RcnR response. Both variants remain unresponsive to Zn(II) binding, and so metal selectivity has not been impaired by the Glu63 alterations. These results indicate that mutation of Glu63 affect the metal site structure, which correlates with a transcriptional effect. In the case of Ni(II), the decrease in transcriptional activity is not affected by the type of mutation, while in the case of Co(II), only the cysteine mutation exhibits a functional effect. These results also indicate that while Glu63 may be involved

in ordering the Zn(II) site, this residue imparts no obvious change to WT-RcnRs response to binding Zn(II).

3.3.5 Circular Dichroism (CD) and Size Exclusion Chromatography (SEC)

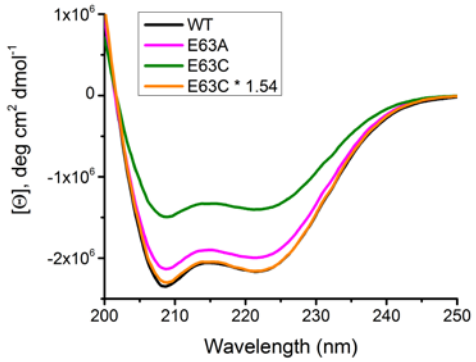

Figure 3.8: CD spectra of apo WT-, E63A-, and E63C-RcnR proteins.

Changes to the secondary structure of RcnR in variants of Glu63 were assessed using circular dichroism. In all cases the spectra are dominated by features at 208 nm and 222 nm which correspond to α-helices and is in line with previous research (**Figure 3.8**).[1] The spectrum of E63C-RcnR appears to be less intense than WT-RcnR, but multiplication by 1.54 (**Figure 3.8**) reveals that the overall line shape is unchanged and this difference in intensity is most likely caused by differences in protein concentration. This does not rule out possible changes in secondary structure, although no features pertaining to other secondary structures are visible. Compared to WT-RcnR, there is no observed change in the CD spectrum of the variants upon the addition of Co(II) or Ni(II) (**Appendix A, Figure A.2**). No change in quaternary structure was observed by size exclusion chromatography (**Figure 3.9** and **Table 3.3**), as all proteins were found to be tetrameric.

Table 3.3: Theoretical and experimentally derived molecular weights as determined by SEC.

Sample	Theoretical MW (kDa)	Experimental MW (kDa)	Quaternary Structure
WT-RcnR	40.0	43.7	Tetramer
E63A-RcnR	39.8	43.7	Tetramer
E63C-RcnR	39.9	49.2	Tetramer

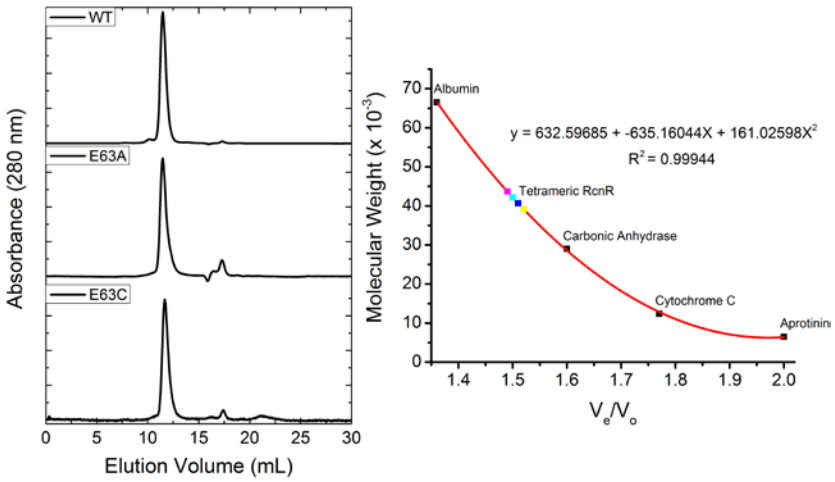

Figure 3.9: (Left) SEC chromatogram of apo WT-, E63A-, and E63C-RcnR proteins in 20 mM HEPES, 150 mM NaCl, 5 mM EDTA,1 mM TCEP, 10 % glycerol, pH 7.0 (Right) Retention volume versus molecular mass for the standards and RcnR proteins. The green dot represents WT-RcnR, the blue dot represents E34A-RcnR, the cyan dot represents E34C-RcnR, the pink dot represents E63A-RcnR and the yellow dot represents E63C-RcnR. The red line represents a second order polynomial fit for the standards.

3.3.6 Fluorescence Anisotropy

The Glu63 mutations showed diminished transcriptional response to the addition of Ni(II) and Co(II). In order to ascertain if this was due to increased DNA-binding affinity, fluorescence anisotropy measurements were performed. 5-carboxytetramethylrhodamine (TAMRA) labeled Site-2 DNA, containing one of two recognition sequences,[18] was titrated with WT-, E63A-, and E63C-RcnR. The apparent K_{DNA} of WT-RcnR is 13.64 nM with no change in the apparent K_{DNA} of either mutant (20.75 nM for E63A RcnR and 17.02 nM for E63C-RcnR) (**Figure 3.10**). This indicates that the E63A and E63C mutationsmutations did not alter DNA binding affinity of the apo-RcnR variants

compared to WT, and therefore the decrease in metal-induced transcriptional responses are independent of DNA-binding affinity.

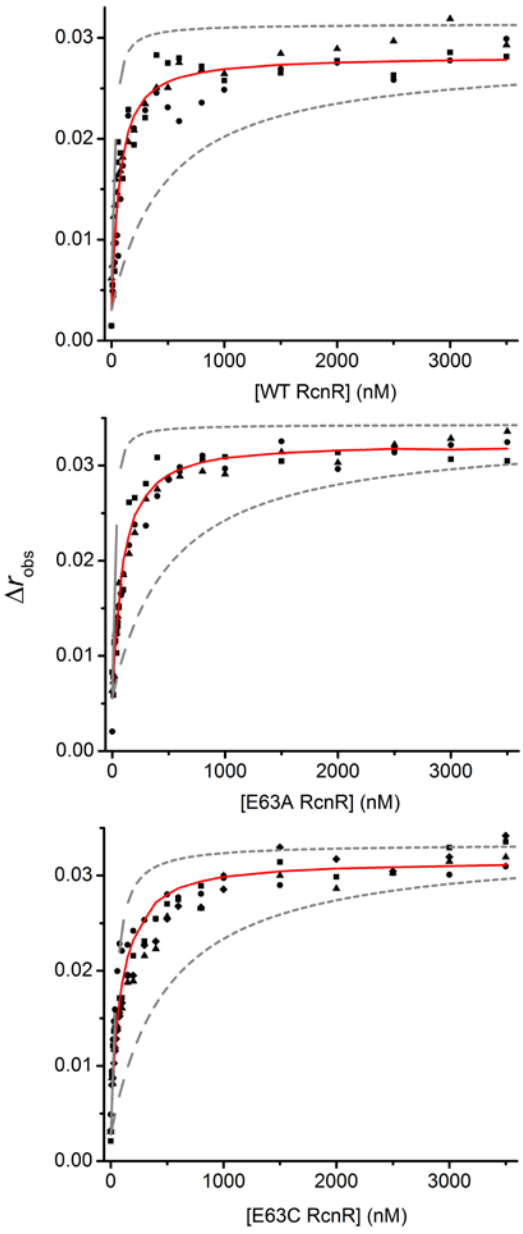

Figure 3.10: Anisotropy changes that occur upon titration of *rcnRS1* (10 μM) with apo WT-RcnR (Top), E63A- (Middle) and E63C-RcnR (Bottom) variants (protomer concentration stated). The experiment was performed aerobically in the presence of 1 mM TCEP and 5 mM EDTA. Symbol shapes represent individual experiments and solid red line represents a simulated curve produced from an average K_{DNA} determined across experiments shown. Dashed lines represent simulated curves with K_{DNA} 10-fold tighter or weaker than the optimized value.

3.4 Results Summary

The XAS results for loss of ligand (E63A-RcnR) and ligand substitution (E63C-RcnR) variants of RcnR give unambiguous structural results for all three metals, Co(II), Ni(II), and Zn(II), and associate Glu63 with metal binding in all cases. In the case of Co(II) E63A-RcnR, a bromide from the solvent replaces one of the N/O-donor ligands. This is most likely due to a vacant first-coordination position around the Co(II) center, consistent with the loss of a ligand (Glu63). In the E63C-RcnR mutation, one of the N/O-donor ligands surround the Co(II) center replaces an S-donor ligand. As there are only two cysteines in the protein, and the buffer consists of Br^- ions instead of Cl^- ions, the only explanation is that the second S-donor ligand comes from Glu63Cys. These two results taken together indicate that Glu63 is clearly a Co(II) ligand in RcnR. This indicates that in addition to Glu34, Glu63 is also a Co(II) ligand. This completes the coordination sphere for Co(II), which has now been shown to bind the N-terminus, His3, Glu34, Cys35, Glu63, and His64 (**Figure 3.11**).[19,20]

In the case of Ni(II), the alteration of Glu63 to Ala results in a six-coordinate Ni(II) center, with one N/O donor replaced by a bromide from solvent, which indicates that the mutation generated an open coordination position around the Ni(II) site and clearly identifies E63 as a Ni(II) ligand. The structure of the Ni(II) complex of E63C-RcnR is similar to the structure found for Ni(II) E34C-RcnR--a 5-coordinate structure containing two S-donor ligands. The Evans method experiment showed that this is a mixture of a ~80% diamagnetic square-pyramidal species and ~20% of a paramagnetic octahedral species.

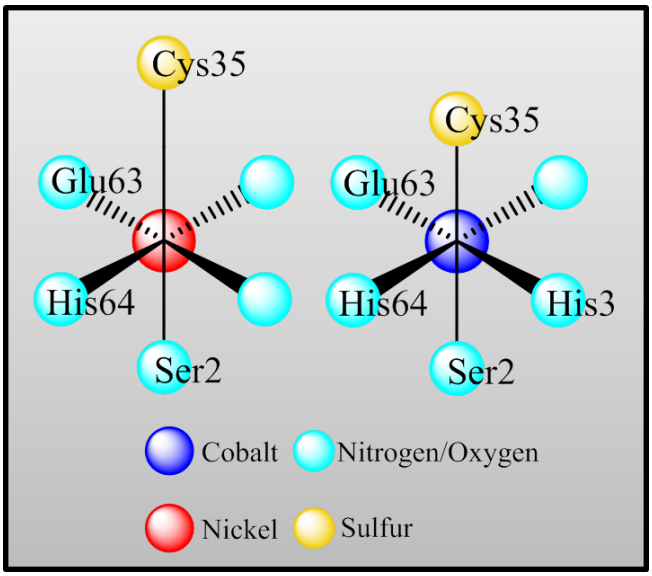

Figure 3.11: New schematic of the metal site structure of Ni(II) and Co(II) with known metal binding residues identified.

In contrast to Glu34, where variants exhibit no change in transcriptional response, Glu63 is more important for the allosteric response of RcnR upon cognate metal binding. For E63A-RcnR, the response to Co(II) binding is WT-like and the response to Ni(II) binding is reduced by 50%. The E63C-RcnR variant demonstrates a reduced Ni(II) response. However, the Co(II) response is also reduced to ~75% of WT-RcnR. It is unclear why a ligand substitution mutation would be more detrimental than a loss of ligand mutation.

3.5 Discussion

Unlike the Glu34 mutations, the Glu63 mutations show a strong correlation between structure and function. These results are in line with previous literature, which show that many metalloregulators utilize first coordination sphere ligand type and geometry to impart functional response and metal selectivity. Coordination number has

been shown to be important in the case of Fur, NikR, and CopY in which the cognate metal (Fe(II), Ni(II), and Cu(I), respectively) adopts a coordination number and geometry that is distinct from non-cognate metals.[21,22] In the case of NmtR, it has been shown that cognate metals Ni(II) and Co(II) adopt six-coordinate geometries and non-cognate metals adopt geometries with lower coordination numbers.[23,24] In the case of SmtB (Zn(II) responsive), and CzrA (Co(II) and Zn(II) responsive), which are part of the ArsR/SmtB family, they bind their cognate metals in a tetrahedral geometry and utilize different ligand sets. The different ligand sets may explain why SmtB is not Co(II) responsive.[24]

The studies on the Glu34 and Glu63 mutations reveal two separate behaviors that would not be revealed without extensive study. Poorly studied metalloproteins may lead to an incomplete picture of or miss-assigned protein function. The dangers of this can be seen clearly in the studies of InrS, a Ni(II) responsive transcriptional regulator in the CsoR/RcnR family, which appears to be poorly metal selective *in vitro*. Only by testing the functional response of InrS in its native organism *Synechocystis* against the complement of metal trafficking proteins was its *in vivo* function elucidated. Further discussion on the relation of the studies outlined in Chapter 2 and Chapter 3 to the CsoR/RcnR family of transcriptional regulators and future studies are outline in Chapter 4.

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CHAPTER 4

CORRELATION BETWEEN FIRST COORDINATION SPHERE AND FUNCTION IN METALLOREGULATORS

4.1 Summary

Chapters 2 and 3 described studies revealing a lack of correlation between structure and function with ligation of Glu34, found to be a ligand for Co(II), and Glu63, a Co(II) and Ni(II) ligand (**Figure 4.1)**. Mutation of either glutamate residue alters the metal site structure, but only mutation of Glu63 affects both structure and transcription for both metals.

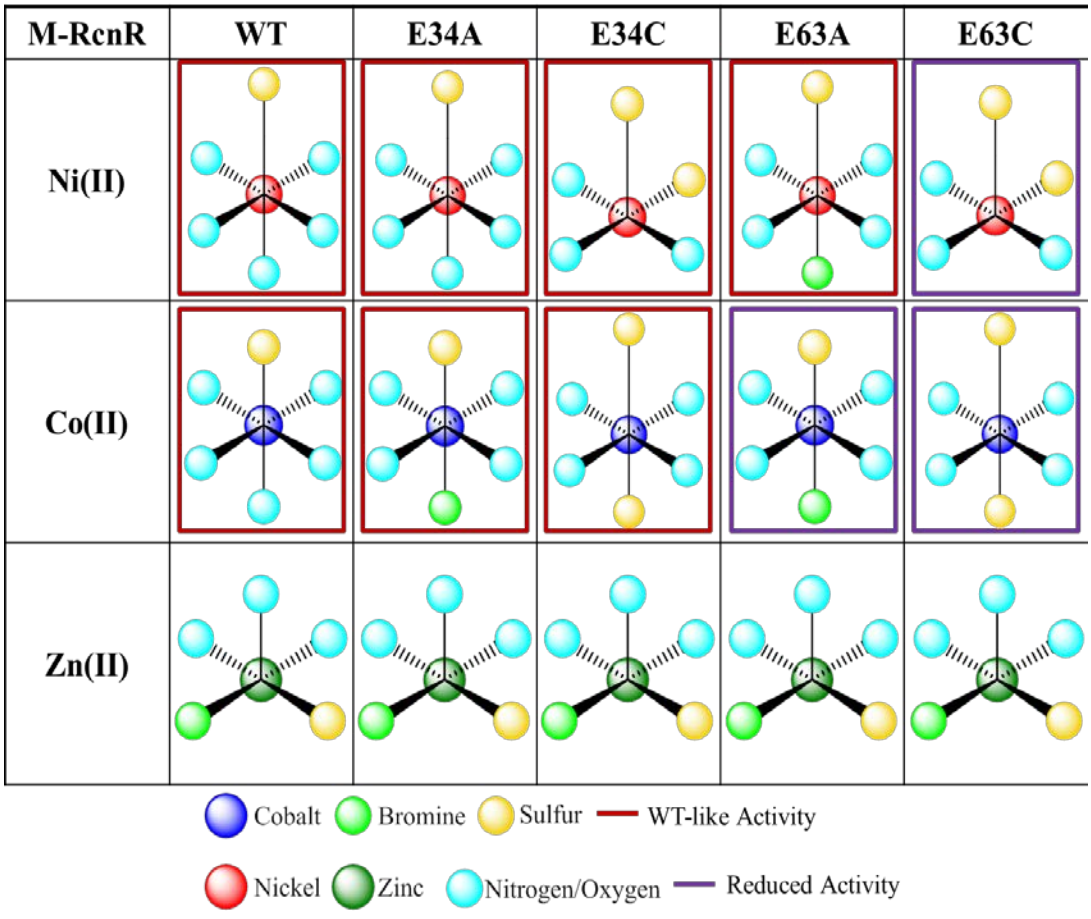

Figure 4.1: Summary of structural and functional changes of the glutamate mutants.

4.2 Conclusions

The relationship between metal selectivity and primary coordination sphere is not clear. While the discussion below will be focused primarily on first coordination sphere, it cannot be disputed that the second coordination sphere is critical for function and is often overlooked. This can be seen in the MerR family of transcriptional regulators, as it has been shown that the metal selectivity of monovalent versus divalent cations and between different pools of monovalent and divalent cations is conferred by tuning the metal environment through second coordination sphere ligands and not through the first coordination sphere.[1] In addition, the importance of the second coordination sphere in proteins is critical in the SOD family of proteins, and is discussed in Section 6.2.3 and is highlighted in the studies on NiSOD discussed in Chapter 7.

Previous literature utilized the so called W-X-Y-Z fingerprint region of the CsoR/RcnR family of transcriptional regulators to determine metal selectivity. Metal selectivity was previously based on a sequence alignment of the identified members of the CsoR/RcnR family with only CsoR and RcnR studied in any detail. Two recently published papers have performed phylogenetic analysis and sequence alignments of all currently identified members of the CsoR/RcnR family.[2,3] These alignments reveal no clear distinction between the amino acids in the canonical W-X-Y-Z fingerprint region[3] that has been used to denote first coordination sphere residues of this family for Ni(II) and Cu(I) sensors. The Ni(II) sensor InrS[2,4] has the same fingerprint motif as the Cu(I) binding proteins in the family, and a different motif than the other known Ni(II) responsive protein, RcnR. Fingerprint analysis, and thus first coordination sphere ligand type, of this family of regulators is obviously a poor way to identify metal responsiveness, an observation previously made by Foster *et al.*[2] Obviously experimentation must occur in order to determine which metals the metalloregulator responds to.

However, identifying the cognate metal of a metalloregulator by structural determination has also been shown to be insufficient, as *Sy*InrS and *Ec*RcnR both respond to Ni(II) binding but bind Ni(II) in four-coordinate planar and octahedral geometry, respectively.[5,4] The role of protein-metal interactions in *in vitro* studies is further confounded by the lack of biological context. Studies of InrS and NmtR reveal that in some cases cognate metals are at least partially dictated by the metal availability inside the cell, which is different for every organism.[4,6]

Based on this knowledge, there is no current way to determine which metal a regulator responds to or how it functions without performing functional experiments in the native organism. The native organism is key, as InrS is not metal selective, but is prevented from binding non-cognate metals by the full complement of cellular trafficking proteins in *Synechocystis*. The trafficking proteins in another organism may have different affinities and mechanisms leading to incorrect functional conclusions. For example, if InrS were tested in *E. coli*, zinc trafficking systems in *E. coli* are not sufficient to prevent RcnR Zn(II) binding and would not be sufficient to prevent Zn(II) binding to InrS. The three most studied members of the RcnR family have three different mechanisms, with RcnR utilizing one or two ligands to act as a 'switch' (section 2.5), CsoR requiring a specific ligand set and coordination (Cys_2His), and InrS exhibiting low metal selectivity *in vitro* in the absence of the total cellular complement of trafficking proteins.

The different mechanisms of action and low sequence identity (~30%) coupled with their widely diverse substrates (Cu(I), Ni(II), Co(II), HSSR, CH_2O) in this class of proteins is indicative of convergent evolution, not divergent. A recent paper suggests these proteins may have evolved at least twice.[7] Their mechanistic difference may be due to a difference in cellular makeup. InrS has poor metal selectivity *in vitro*, but *in vivo* the full complement of metal

trafficking proteins neutralizes this issue, indicating proteins like InrS never developed metal selectivity because of the lack of necessity to do so. In the case of CsoR, the Cys_2His Cu(I) binding site has been found in a variety of proteins and is thought to change both protein-protein interactions and the metal transfer chemistry.[8–12] As a terminal metal acceptor, changes in protein interactions and metal transfer would disfavor transfer of metal from CsoR to other Cu binding proteins having higher affinity and the common Cys_2/Cys_3 Cu(I) binding sites. This change is seen in *Streptomyces* CsoR, which demonstrates an affinity for Cu(I) ions identical to chaperone CopZ with a unidirectional Cu(I) transfer to CsoR. For RcnR, the purpose of the switch mechanism could be due to the binding of non-cognate metals. It has been previously shown that Zn(II), Cu(I) and Cu(II) all bind to the same relative site on the protein as the cognate metals Ni(II) and Co(II).[5,13,14] In the case of H3E, which gained partial Zn(II) activity,[13] the β-galactosidase results indicate that the Zn(II) trafficking system is not sufficient to keep metal away from RcnR, as it is for InrS in *Synechocystis*. If most or all of the ligands are required for function as has been previously hypothesized, than it is possible that noncognate metals could at least partially activate RcnR. However, if the 'switch' is the one or two ligands that are not bound by noncognate metals than binding to RcnR will not cause release from DNA.

Although RcnR does not appear to operate in a manner similar to InrS, the cellular trafficking system also affects its function, at least in the case of Ni(II). Change in the function of Ni(II) exists in β-galactosidase metal titration activity assays in which WT-RcnR responds to Co(II) at a much lower concentration than Ni(II). This is most likely due to Ni(II) availability in the cell. Previous studies have shown that WT-RcnR has similar affinities for both Ni(II) and Co(II) (~100 nM) *in vitro,*[5] indicating that WT-RcnR should respond to both at the same concentration all things being equal. However, *E. coli* has no known use for Co(II) which is a

highly toxic metal, while it has a dedicated Ni(II) trafficking system in order to facilitate maturation of the three [NiFe]-hydrogenase enzymes. In this case, the rest of the trafficking system (NikABCDE, NikR, HypA, HypB, SlyD) and the target enzymes must have their Ni(II) requirements met before RcnR activation for Ni(II) export. It is likely that RcnR, and by relation RcnAB, is the last protein to obtain Ni(II) in the system. This may also prevent Ni(II) deficiency, as the *rcn* operon is often transcribed in the presence of Co(II) at low cellular concentrations. This may also explain why RcnB was shown to reduce the export of Ni(II) and Co(II) by RcnA.[15,16] If there is always at least a small amount of *rcnAB* then there might be Ni(II) depletion in the cell if RcnA is always continuously exporting Ni(II).

4.3 Future Directions

As outlined above, the W-X-Y-Z fingerprint region is insufficient for determining metal selectivity in this family of transcriptional regulators. However, metal site structure determination and standard β-galactosidase functional analysis alone is also insufficient. The matter is also complicated by the diversity in this family. So far, the three most well studied members of this family have displayed diverse mechanisms in terms of metal selectivity, even when regulating identical metals (RcnR and InrS). A second metalloregulator exists for Cu(I), RicR, but whether RicR functions through the same mechanism has not been determined. However, Ni(II) regulation in this family displays the best chance of understanding whether these mechanisms are widespread.

4.3.1 Determination of First Coordination Sphere Geometry of the metal site in DmeR by XAS

Recently, a new Ni(II) and Co(II) regulator in this family, DmeR from *Rhizobium leguminosarum*, was characterized.[17] DmeR regulates itself and DmeF, a Ni(II) and Co(II) exporter protein. Because DmeR was shown to respond to both Ni(II) and Co(II), it provides an excellent example to determine if it regulates its cognate metals utilizing the same ligand set as RcnR. Similar to RcnR, DmeR has only one cysteine which aligns with the strictly conserved Cys35 (RcnR numbering) that all members of this family contain. DmeR has a histidine in position 3, similar to RcnR, as well as a histidine in position 64 (RcnR numbering). DmeR does not have glutamate residues in position 34 or 63. Determining purification protocols for DmeR is the first step, as it has only been studied functionally in its native organism. Studying DmeR via XAS when bound to Co(II), Ni(II), and Zn(II) to determine first coordination sphere geometry and ligand type would further understanding of the distribution of metal structures across this family of transcriptional regulators. The next step would be to determine function of this protein in its native organism. It was previously determined that DmeF exports Ni(II) and Co(II) and thus assumed that DmeR also responds to these metals. β-galactosidase functional studies and RT-PCR in *Rhizobium leguminosarum* are necessary to provide a more direct measurement of DmeR response to these cognate metals. The *in vivo* functional analysis coupled with *in vitro* metal selectivity through competition assays or ITC would also give a better understanding if the mechanism of DmeR is more in line with RcnR or InrS without identifying and studying the entire trafficking compliment of *Rhizobium leguminosarum.*

4.3.2 Determination of First Coordination Sphere Geometry of the metal site of NcrB by XAS

Ni(II) regulation affords the best way to study the mechanisms of metal regulation in this family because of the diversity of and sequence of identified Ni(II) regulators. In addition to

DmeR (section 4.3.1), another Ni(II) regulator NcrB from *Leptospirillum ferriphilum* has been discovered. NcrB regulates NcrA and NcrC, which are membrane proteins that form an efflux system (section 1.4.8). NcrB has not been tested for responsiveness to a metal other than Ni(II). The NcrB sequence is most similar to InrS, and contains an H-C-H-C 'fingerprint' in the same positions as InrS. NcrB lacks the histidine rich tail of InrS, so that its only N-terminal histidine aligns with His3 of RcnR. Studying both the first coordination sphere of the protein bound to Ni(II), Co(II), and Zn(II) by XAS would provide a better understanding of this family of regulators. Functional studies utilizing β-galactosidase transcriptional assays as well as RT-PCR would provide a better understanding of the metals that NcrB responds to and the cellular concentration at which it is active. However, if NcrB does indeed function in a similar manner to InrS, its true cellular function would only be understood if the functional studies were performed in the native organism *Leptospirillum ferriphilum*. This protein would first need a purification protocol as the original paper purifies via a His-tag but does not cleave it and this may interrupt function based on studies of RcnR. As with DemR, *in vitro* metal selectivity via competition assays or ITC would also provide a better understanding of the mechanism of NcrB in relation to RcnR and InrS. This protein contains an H-C-H-C fingerprint region, similar to InrS and CsoR from *Thermus thermophilus*, both of which have displayed promiscuity in their metal selectivity. The β-galactosidase experiments or EMSA (electrophoretic mobility shift assays) would be able to test for promiscuity in metal binding and could be done in conjunction with Future Directions 4.3.4 to determine if this H-C-H-C fingerprint region imparts or is related to a specific mechanism rather than metal selectivity.

4.3.3 Determine whether YrkD is a RcnR/CsoR family member.

YrkD is an uncharacterized protein that is presumed to be a member of this family of regulators based on its homology. It contains many of the highly conserved residues within this family which supports its inclusion. It is also the second most widely distributed protein in the family, only slightly behind CsoR. Due to its presence in *Mycobacterium tuberculosis*, which already has two Cu(I) responsive regulators from this family, it is extremely unlikely that it is a Cu(I) binding protein despite YrkD having two highly conserved cysteines in the same positions as CsoR. Other than this, it lacks any and all conserved metal binding residues and lacks histidines of any sort. This makes classifying this protein especially interesting. The most obvious starting place would the YrkD gene from *M. tuberculosis*, not just because this organism already has Cu(I) binding proteins and YkrD has a Cu(I) binding motif (Cys_2) but because this is the most well understood organism that this protein has been found in. The first step is to inspect the genes to either side of *yrkD* and see if they are homologous to known metal exporters. In addition, examination of the intergenic regions for a palindrome or repeat sequence is necessary. Purification of YrkD would be necessary and DNA binding experiments done to determine if it binds to any determined palindrome or repeat sequences with high affinity (~100 nM). This can be done with electrophoretic mobility shift assays (EMSA) or fluorescence anisotropy. In the case of DNA binding, EMSA can also be used in conjunction with metals to determine if metal can reverse DNA binding. Obviously, once it has been confirmed to bind to a DNA sequence, RT-PCR should be performed to see if transcript levels corresponding to exporter proteins, or proteins on the same operon as YrkD, are affected by metal addition. Once these experiments are done, there should now be a basis for performing XAS on YrkD bound to various metals (Ni(II), Co(II), Cu(I), Zn(II)).

4.3.4 Test *D. radiodurans* CsoR for metal responsive promiscuity.

InrS has a W-X-Y-Z fingerprint of H-C-H-C which aligns with the CsoR from *Thermus thermophilus*. Both of these regulators have shown promiscuity in the metals they respond to *in vivo*, suggesting that although they respond to different metals they function by similar mechanisms, where the cellular complement of metalloregulators are sufficient to prevent non-cognate metals from binding these regulators. Interestingly, CsoR from *D. radiodurans* has a H-C-H-C fingerprint, but was not tested for any metals beyond Cu(I). β-galactosidase transcription reporter assays or EMSA should be performed after metal addition to determine if *D. radiodurans* CsoR is promiscuous, as this would implicate the H-C-H-C fingerprint as imparting a specific mechanism rather than metal selectivity. XAS should be done in conjunction with β-galactosidase transcription reporter assays or EMSA to determine if the CsoRs from *T. thermophilus* and *D. radiodurans* bind Cu(I) in a trigonal planar or four-coordinate planar geometry. Although the currently studied CsoRs bind Cu(I) in a trigonal planar geometry, they lack the H-C-H-C motif. In addition, as seen in Chapter 5, InrS binds Cu(II) in a four-coordinate planar geometry and this coordination may be due to the W-X-Y-Z binding motif. In addition, XAS should be done on other metals implicated in the EMSA assay to determine their coordination number to compare the coordination of cognate versus non-cognate metals. If these CsoRs are promiscuous, non-cognate metals may adopt coordination numbers similar to the cognate metals, as seen in studies of InrS.

4.4 References

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CHAPTER 5

INVESTIGATION INTO THE FIRST COORDINATION SPHERE OF THE INRS NI(II) SITE

5.1 Introduction

InrS is a Ni(II) responsive metalloregulator in *Synechocystis* (see section 1.4.3). The so-called 'W-X-Y-Z fingerprint' region of InrS is H-C-H-C, which aligns with the Cu(I) responsive regulator, CsoR, and not with the other known Ni(II) regulator RcnR.[1] Because InrS is the third member of this family to be characterized, it was proposed that analysis of the fingerprint region is a poor way to determine what metal the protein responds to.[1] In addition, InrS was shown to have a four-coordinate planar geometry by UV-Vis, with a tentative assignment of two sulfur ligands, which is distinct from RcnR which is octahedral and binds one sulfur ligand.[2] Thus it is clear that this family of metalloregulators, which all have approximately the same secondary and quaternary structure and share ~30% identity, can perform similar functions with very different ligand environments. All current members of the RcnR/CsoR family bind the residues in the X-Y-Z positions of the fingerprint region in their first coordination sphere.[3] Thus, Cys36, His61, and Cys65 of InrS were proposed to be metal binding residues and this was supported by X-ray crystallography of apo-InrS, which revealed that the two cysteines within the protein are directly opposite one another, with His61 immediately adjacent (unpublished data).[4] The fourth ligand is unknown, but InrS has an N-terminal tail that is rich in histidines. His21 of InrS aligns with His3 of RcnR, known to be a first coordination sphere ligand for Co(II) and involved in metal responsiveness for Ni(II). Thus, it was proposed that His21 is a ligand for InrS.[1,5]

To more definitively characterize the metal site structure of InrS, XAS was done on InrS bound to Ni(II) in buffer containing NaBr or NaOAc. Because InrS is Cu(II) responsive *in vitro*, XAS was performed on InrS complexed to Cu(II) to determine whether or not it occupied the same site as Ni(II) which would provide a basis for this responsiveness. Lastly, H21L-InrS complexed to Ni(II) was investigated by XAS to see if a change in the first coordination sphere could be detected, providing basis for H21 as the fourth ligand completing the coordination sphere of InrS.

5.2 Experimental Procedures

5.2.1 X-ray Absorption Spectroscopy

Samples were prepared by collaborators in Dr. Nigel Robinson's lab according to a published procedure.[6,7] Samples of 1 - 2 mM metal were prepared in 10 mM HEPES, pH 8.1, 1 M NaBr, 5 mM TCEP and metal concentration was determined by ICP-MS by Dr. Andrew Foster. XAS was also done on a sample of Ni(II) WT-InrS in buffer containing 1 M NaOAc instead of NaBr.

Data collected at NSLS used samples that were cooled to ~30 K using a He displex cryostat under ring conditions of 2.8 GeV and 120-300 mA, with a sagittally-focusing Si(111) double-crystal monochromator. X-ray fluorescence was collected using a 30-element Ge detector (Canberra). Scattering was minimized by placing a Z-1 filter between the sample chamber and the detector. An internal energy calibration was performed by collecting spectra simultaneously in transition mode on the corresponding metal foil to determine the first inflection point on the edge, which was set to 8,331.6 (Ni) or 8,980.3 eV (Cu). X-ray absorption near-edge structure (XANES) data were

collected from -200 to +200 eV relative to the metal K-edge. Extended X-ray absorption fine structure (EXAFS) data were collected to 15 *k* above the edge energy (E_0). Because the Cu(II)-InrS sample was photo-reduced in the beam based on a >0.8 eV shift in edge energy between two successive scans, one batch of InrS was split into two samples. During data collection each sample was moved after each scan so that the incident X-ray beam irradiated a new section of sample to obtain the spectrum of the Cu(II) complex. This yielded 8 scans that were analysed for changes in edge energy. Finding no changes in energy they were then averaged.

The Ni(II)-H21L sample was run on beam line 7-3 at SSRL. The data were collected at ~10 K using a liquid helium cryostat (Oxford Instruments) under ring conditions of 3 GeV and 495-500 mA. Beam line optics consisted of a Si(220) double-crystal monochromator and a flat rhodium-coated mirror before the monochromator for harmonic rejection and vertical collimation. X-ray fluorescence was collected using a 30-element Ge detector (Canberra). Soller slits with a Z-1 element filter were placed between the sample chamber and the detector to minimize scattering.

5.2.2 Data Reduction and Analysis

The SixPack software[8] program was used to remove bad channels, average the data, and to perform energy calibrations, in addition to data reduction and normalization. Background correction was performed using a Gaussian pre-edge function and a quadratic polynomial for the post-edge region followed by normalization of the edge jump. A seven section, fourth-order polynomial spline between k = 2 Å^{-1} and k = 14 Å^{-1} was used for EXAFS baseline correction. The Artemis software program was used for

EXAFS analysis by utilizing the EXAFS equation with parameters generated using FEFF6.[9,10] The EXAFS equation is defined as:

$$\chi(k) = \sum_i \frac{N_i f_i(k) e^{-2k^2\sigma_i^2}}{kr_i^2} \sin[\,2kr_i + \delta_i(k)]$$

where *f(k)* is the scattering amplitude, *δ(k)* is the phase-shift, *N* is the number of neighboring atoms, *r* is the distance to the neighboring atoms, and σ^2 is the disorder to the nearest neighbor. The data were converted to *k*-space using the $k = [\frac{2m_e(E-E_0)}{\hbar^2}]^{1/2}$ relationship, where m_e is the mass of an electron and $\hbar$ is Plank's constant divided by 2π. All data sets were Fourier-transformed using a Kaiser-Bessel window over the range k = 2 – 14 Å, and fit as previously described in *r*-space over the range r = 1 – 4 Å in order to assess multiple-scattering contributions from histidine imidazole rings, and employing an amplitude reduction factor (S_0) value of 0.9. The reported Fourier-transformed spectra were not phase-corrected. Reported data sets were fit with separate sets of Δr_{eff} ($r - r_{eff}$) or the change in metal-ligand bond distance with respect to the input path distance) and σ^2 for the sulfur and nitrogen-donors including imidazole rings with initial values of 0.0 Å^2 and 0.003 Å^2, respectively. Each fit was initiated with a universal E_0 (8,340 eV for Ni and 8,990 eV for Cu) and ΔE_0 = 0 eV, which was allowed to vary for each fit. Histidine ligands were fit as geometrically rigid imidazole rings with varied angles of rotation (α), with α being defined as the rotation around an axis perpendicular to the plane of the ring and going through the coordinated nitrogen. The distances of the five non-hydrogen atoms in the imidazole ring were fit in terms of a single Δr_{eff} for various angles (0 – 10°) so that all atoms in the ring move with the Ni(II)-N distance.[11–13] Multiple-scattering parameters for imidazole ligands bound to Ni(II) and Cu(II) were generated using the

FEFF6 software package with the imidazole input obtained from average bond lengths and angles gathered from crystallographic data, as previously described.[14,15] All multiple scattering paths with path lengths outside the fitting window (r = 1 – 4 Å) were discarded. Histidine 'counting' was performed by adding integer numbers of histidine imidazole ligands to fits and assessing the effect on the *R*-factor and reduced χ^2.

To assess the goodness of fit from different fitting models, the fit parameters χ^2, reduced χ^2 (*red* χ^2), and *R*-factor were minimized. Increasing the number of adjustable parameters is generally expected to improve the *R*-factor; however χ^2 may go through a minimum, with the increase indicating the model is over-fitting the data. These parameters are defined as follows:

$$\chi^2 = \frac{N_{\text{idp}}}{N_{\varepsilon^2}} \sum_{N}^{i=1} \left(\text{Re}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2 + \text{Im}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2 \right)$$

And

$$red\chi^2 = \frac{\chi^2}{N_{\text{idp}} - N_{\text{var}}}$$

Where N_{idp} is the number of independent data points defined as $N_{\text{idp}} = \frac{(2\Delta r \Delta k)}{\pi}$, Δr is the fitting range in *r*-space, Δk is the fitting range in *k*-space, N_{var} is the number of refining parameters and represents the degrees of freedom in the fit, N_{ε^2} is the number of uncertainties to minimize, Re() is the real part of the EXAFS Fourier-transformed data and theoretical functions, Im() is the imaginary part of the EXAFS Fourier-transformed data and theoretical functions, and $\tilde{\chi}(R_i)$ is the Fourier-transformed data or theoretical function.

Additionally, IFEFFIT calculates the R-factor for each fit, which is directly proportional to χ^2 and a measure of the absolute misfit between the data and theory given by:

$$\boldsymbol{R} = \frac{\sum_{i=0}^{n}\{\mathrm{Re}[\tilde{\chi}_{data}(R_i) - \tilde{\chi}_{theory}(R_i)]^2 + \mathrm{Im}[\tilde{\chi}_{data}(R_i) - \tilde{\chi}_{theory}(R_i)]^2\}}{\sum_{i=0}^{n}\{\mathrm{Re}[\tilde{\chi}_{data}(R_i)]^2 + \mathrm{Im}[\tilde{\chi}_{data}(R_i)]^2\}}$$

5.3 Results

5.3.1 XANES analysis

Analysis of the XANES spectrum yields information on the coordination number and geometry of the metal center. Ni(II) and Cu(II) both exhibit pre-edge features in the XANES that are associated with high-energy electronic transitions. For Ni(II) this usually includes a 1s → 3d transition, which provides a measure of centrosymmetricity, and a 1s → $4p_z$ transition, which is present in the spectra of complexes with geometries that lack one or more axial ligands.[16] All XANES spectra for InrS lack an observable 1s → 3d transition so no peak fitting could be performed. All XANES analysis is based on the presence and resolution of the 1s → $4p_z$ transition. XANES analysis of Ni(II) complexes of WT-InrS and H21L-InrS as well as Cu(II)-complexes of InrS are summarized in **Table 5.1** and shown in **Figure 5.1**.

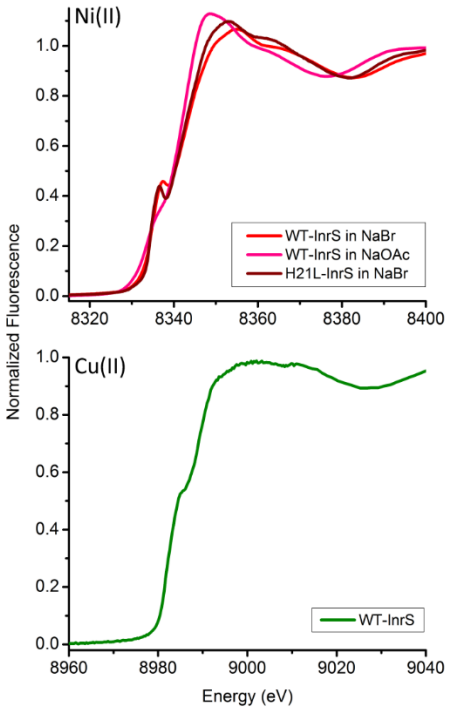

Figure 5.1: *K*-edge XAS spectra of InrS complexed to Ni(II) (Top) and Cu(II) (Bottom) in buffer containing 10 mM Hepes, 1 M NaBr (or 1 M NaOAc), 5 mM TCEP at pH 8.1.

Table 5.1: XANES and EXAFS Analysis for Metal Complexes of WT- and H21L-InrS Mutant Proteins in Buffer with 1 M NaBr.

	XANES Analysis				EXAFS Analysis					
Sample	K-edge energy (eV)	1s → 3d peak area (x10^2 eV)	1s → 4p$_z$ observed	Coord #/geometry	Shell	*r* (Å)	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	%R	rχ^2
				WT-InrS						
Ni(II)	8341.5	<0.5	Yes	4/planar	1 N/O	1.87(3)	2(2)	0(3)	8.9	54.2
					1 S	2.18(3)	1(2)			
					1 S	2.28(3)	2(3)			
					1 Imd0°	1.96(6)	6(7)			
					1 S	**2.18(4)**	**7(6)**	0(2)	4.3	25.9
					1 S	**2.26(3)**	**2(2)**			
					1 Imd0°	**2.02(2)**	**1(1)**			
					1 Imd0°	**1.87(1)**	**1(1)**			
					2 S	2.23(1)	5(1)	2(1)	4.9	23.1
					1 Imd0°	2.02(2)	1(1)			
					1 Imd0°	1.87(1)	1(1)			
Cu(II)	8990.0	<0.5	Yes	4/planar	1 N/O	2.08(4)	2(2)	1(2)	2.6	2.6
					1 S	2.16(3)	5(10)			
					1 S	2.29(2)	1(2)			
					1 Imd0°	2.01(3)	5(3)			
					1 S	**2.19(1)**	**0(1)**	**0(1)**	**1.8**	**6.7**
					1 S	**2.30(1)**	**1(1)**			
					1 Imd0°	**1.99(3)**	**7(3)**			
					1 Imd10°	**2.14(2)**	**3(2)**			

					2 S	2.25(1)	5(1)	1(2)	3.1	10.3
					1 Imd0°	2.06(6)	6(6)			
					1 Imd0°	2.06(14)	13(16)			
Ni(II)	8432.3	<0.5	Yes	5/pyr	**1 N/O**	**2.23(4)**	**9(2)**	**-4(3)**	**4.4**	**199**
					1 S	**2.12(3)**	**1(6)**			
					1 S	**2.24(3)**	**6(3)**			
					1 Imd0°	**1.86(4)**	**4(4)**			
					1 Imd10°	**2.03(2)**	**3(1)**			
					1 S	2.26(1)	4(1)	-5(2)	5.3	196
					1 S	2.11(1)	1(1)			
					1 Imd0°	1.83(2)	3(3)			
					1 Imd10°	2.03(2)	2(2)			
				H21L-InrS						
Ni(II)	8342.3	<0.5	Yes	4/planar	**1 N/O**	**1.86(2)**	**1(1)**	**-1(2)**	**4.1**	**54.0**
					1 S	**2.12(2)**	**3(4)**			
					1 S	**2.24(1)**	**1(1)**			
					1 Imd10°	**2.02(2)**	**1(1)**			
					1 S	2.22(2)	0(1)	-2(2)	4.7	61.0
					1 S	2.16(4)	7(7)			
					1 Imd0°	1.86(2)	0(2)			
					1 Imd0°	1.99(3)	1(3)			
					1 N/O	1.84(3)	3(3)	-3(1)	5.0	57.0
					2 S	2.20(1)	3(0)			
					1 Imd0°	1.90(2)	1(1)			

The Ni(II) WT-InrS complex in NaBr buffer lacks an obvious peak corresponding to a 1s → 3d transition, indicating that the ligands are arranged in a centrosymmetric geometry, such as four-coordinate planar or octahedral. The spectrum additionally exhibits a resolved maximum at ~8,336 eV, which corresponds to a 1s → $4p_z$ transition that is diagnostic for a four-coordinate planar geometry.[16] In the case if Ni(II)-InrS complex in NaOAc buffer there is no observable 1s → 3d transition similar to InrS in NaBr, but the 1s → $4p_z$ transition is a shoulder and not a resolved maximum. This rules out a square-planar geometry, indicating that the buffer has affected the first coordination sphere geometry of InrS, which has been seen previously in XAS studies of RcnR.[6,17] The lack of an observable 1s → 3d is indicative of a centrosymmetric environment although there are no geometries which correspond to an unresolved 1s → $4p_z$ and a small 1s → 3d. It has been previously shown[18] that some square pyramidal geometries have large 1s → $4p_z$ and no measurable 1s → 3d, so Ni(II)-InrS in NaOAc buffer was assigned as

having square-pyramidal geometry, with an acetate from buffer as the axial ligand being the most reasonable assumption. The Ni(II)-H21L complex has similar pre-edge features as the Ni(II)-InrS complex, with no obvious 1s → 3d transition and a resolved 1s → $4p_z$ transition at ~8,337 eV, also indicating a four-coordinate planar geometry.

The Cu(II) pre-edge region is often featureless and is notably insensitive to changes in ligand environment, so assignment of the coordination number is often not possible from XANES analysis.[19–21] The Cu(II)-InrS complex does not exhibit a pre-edge feature corresponding to a 1s → 3d transition. This feature is often absent with Cu(II) due to decreased intensity associated with the d^9 electronic configuration, but is consistent with a centrosymmetric geometry. However, the Cu(II)-InrS spectrum exhibits a low-energy pre-edge tail with a normalised amplitude of 0.39 at 8,384.0 eV, that is associated with a lower energy 1s → 4p transition at 8,986 eV. This is indicative of higher covalency and is only seen in complexes containing two or more S-donor ligands.[20]

5.3.2 EXAFS analysis

Analysis of the EXAFS region of an XAS spectrum yields information on the type of donor atom (Z ± 2) and the distance from the scattering atom (± 0.02 Å), as well as providing a second measure for the coordination number (± ~20 %). XAS cannot differentiate between atom types with Z ± 1, so in buffers containing NaCl it can be difficult to distinguish protein S-donor ligands from Cl^- ligands. For this reason the initial EXAFS data was collected using buffer containing NaBr. The data was first fit with a single shell of N donor atoms with coordination number 4 - 6. Then the data was fit with a single shell of S-donor atoms with coordination number 4 - 6. Neither single shell fit

generated a fit with a % R-value < 5%. The data was then fit with a mixed shell of N and S donors, with all possible combinations of N- and S donors at various distances with CN = 4. This improved the fit, and the best fit ($(N/O)_2S_{2)}$ %R = 14.3) is shown in **Table 5.1**. A mixed shell fit did not result in a fit with a % R-value of < 5%, so scattering from imidazole rings was then addressed, where imidazoles were modelled as rigid rings. The best EXAFS fits (**Table 5.1**), obtained for the Ni(II)-InrS spectrum are four-coordinate, consistent with the XANES analysis, and feature two S-donor ligands and two N/O-donors. The analysis of the coordination sphere of the Ni(II)-InrS site was done with either one shell of two S-scattering atoms, or by refining the two Ni(II)-S distances independently. The latter approach led to one short (2.15(3) Å) and one longer Ni(II)-S distance (2.25(2) Å), the shorter of which is at the lower limit observed for four-coordinate planar thiolates.[69] The difference in the two distances is below the resolution of the data set ($k = \frac{\pi}{2\times\Delta k} = 0.126$) but gives lower values of both the *r*-factor and reduced χ^2 than fits generated with a single shell of S scattering atoms. Refinement as one shell of sulfur fits nearly as well and also results in a reasonable average Ni(II)-S distance for a four-coordinate planar complex (2.23(1) Å). EXAFS analysis of all other spectra were performed in a similar fashion as Ni(II)-InrS (**Table 5.1**).

It is similar to Ni(II)-InrS in NaBr in that there are two S-donor ligands. As InrS has only two cysteines in the protein, and the buffer contains no chloride, this indicates that the Ni(II) is bound in the same position as Ni(II)-InrS in NaBr but with one axial ligand. Multiple scattering was then assessed and the best fit consists of three N/O ligands, two of which are imidazoles, and two S-donor ligands. Thus the Ni(II)-InrS in NaOAc has the same His_2Cys_2 coordination as Ni(II)-InrS in NaBr. The axial ligand may

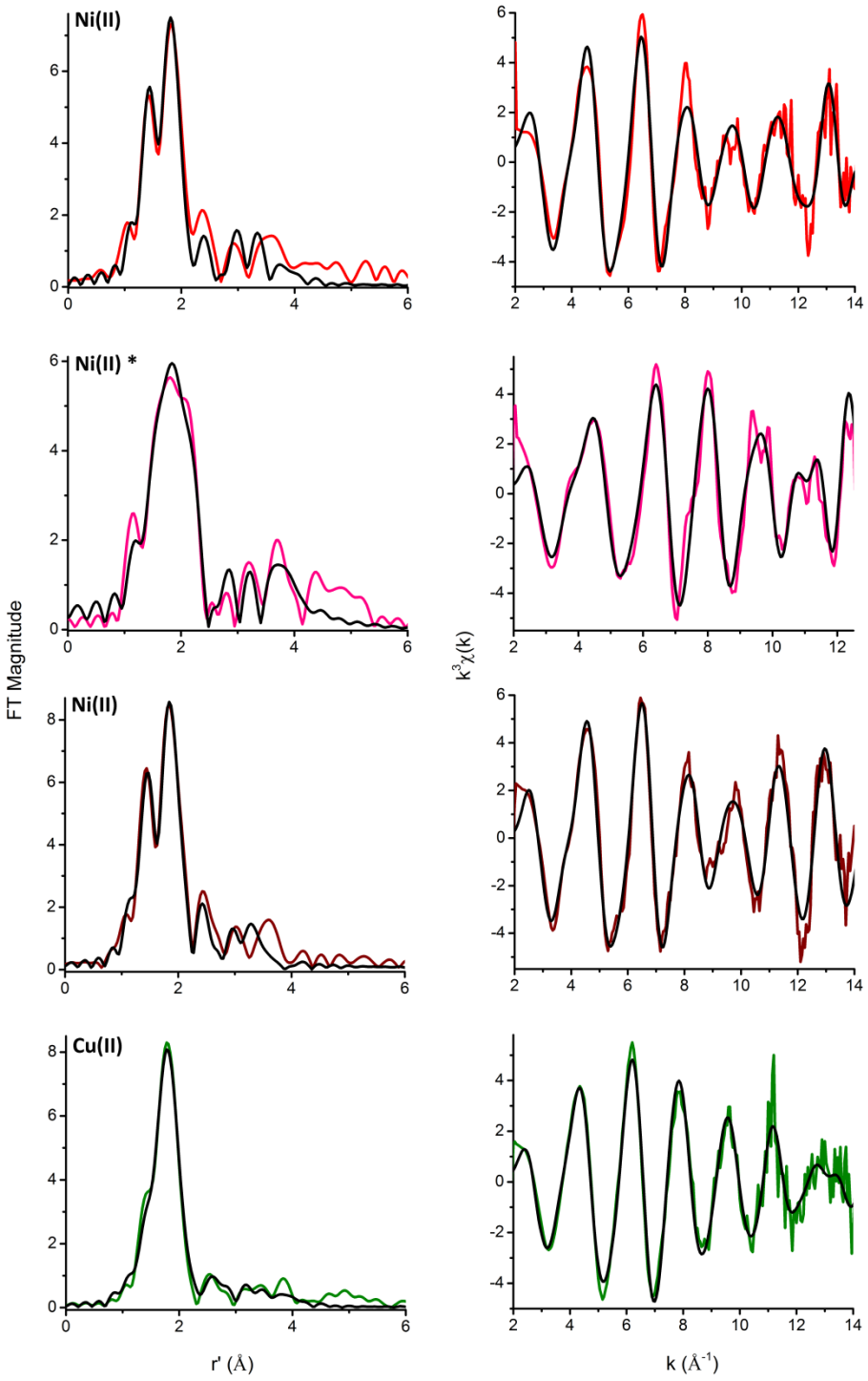

Figure 5.2: K-Edge XAS spectra of WT- and H21L-InrS Ni(II) and WT-InrS Cu(II) complexes in buffer containing 20 mM Hepes, 300 mM NaBr, 1 mM TCEP and 10% glycerol at pH 7.0 and the WT-InrS Ni(II) complex in 300 mM NaOAc buffer (*): (Left) Fourier-transformed EXAFS data (colored lines) and fits (black lines). (Right) Unfiltered k^3-weighted EXAFS spectra and fits.

be a fifth ligand from protein, but it is unlikely that the buffer would so significantly affect the protein structure as to allow another protein residue to bind. Instead, it is most likely an acetate ligand binding axially.

The XANES spectrum for Ni(II)-H21L resembles that of Ni(II)-InrS, and establishes a four-coordinate planar Ni(II) complex for H21L as well. The EXAFS analysis (**Fig. 5.2** and **Table 5.1**) is consistent with the XANES spectrum, with the best fit being four-coordinate. When the data is fit with a mixed shell of N/O and S donors the best fit is ($(N/O)_2S_2$ %R = 9.4), identical to Ni(II)-InrS but with a lower %R, due to the higher contribution of the first shell ligands to the total *r*-space. However, this %R is not < 5%, so multiple scattering from imidazole ligands was assessed for its contribution to the fit. Like InrS, the best EXAFS fits (**Table 5.1**) feature two S-donor ligands at comparable distances (average Ni(II)-S = 2.20(1) Å) and two N/O-donor ligands. However, unlike wild type InrS, the best fit of the H21L variant features multiple-scattering from only one imidazole, consistent with H21 providing the second imidazole ligand in wild type InrS. However, this best fit is not significantly different from the fit with two imidazoles and so whether there are one or two imidazoles present cannot be definitively determined. However, this is in marked contrast to WT-InrS wherein the best fit unequivocally contains two imidazoles. As InrS has an N-terminus with a high histidine content it is possible that one of these histidines has replaced it as a ligand. Notably, there was only a modest change in Ni(II) affinity of H21 variants and it is feasible that optional (redundant) replacement ligands might be recruited by these proteins.

In the case of the Cu(II)-complex, when the data is fit with a mixed shell of N/O and S-donors, the best fit is ($(N/O)_2S_2$ %R = 4.0), which is identical to Ni(II)-InrS. In this case the best fit is < 5%, which is typical of Cu XAS as multiple scattering tends to have low intensity relative to the first shell atoms. However, there are obvious features in *r*-space between 3 – 4 Å, so contributions from multiple scattering by imidazoles was assessed. The EXAFS spectrum of the Cu(II)-complex of InrS is similar to that of the Ni(II) complex (**Fig. 5.2** and **Table 5.1**), with the best fit being four-coordinate and featuring two S-donor ligands and two imidazole ligands derived from histidine residues. The identical geometry and ligand types indicate that Cu(II) occupies the same binding site as Ni(II).

5.4 Conclusion

WT-InrS bound to Ni(II) was previously characterized by UV-Vis as being four-coordinate planar, with a S→Ni(II) CT band with an intensity that is indicative of two sulfur atoms.[2] XANES analysis of this complex supports a four-coordinate planar geometry, and EXAFS analysis confirms the presence of two sulfur ligands which presumably come from the only two cysteines in InrS. In addition to two S-donor ligands, the coordination sphere of InrS is completed by the side chain imdazoles of two histidine ligands. One of these histidines is proposed to be His61, as it aligns with a metal binding residue in RcnR and all currently characterized CsoRs. The second histidine studied in this work is H21L, which aligns with His3 in RcnR and is a Co(II) binding residue.[6] XANES analysis of WT-InrS in NaOAc buffer gave a five-coordinate pyramidal geometry as being the most plausible, indicating that a change in geometry has occurred

due to solvent effects. EXAFS analysis revealed a fit identical to Ni(II) WT-InrS in NaBr buffer except for an additional N/O ligand, most likely an axially bound acetate molecule. This confirmed the assignment of WT-InrS in NaBr complexed to Ni(II) having a His_2Cys_2 ligand set which is solvent exposed.

InrS was previously shown to be promiscuous, responding to a variety of metals *in vivo*.[1,2] The XAS study on Cu(II) provides an explanation for this promiscuity, as WT-InrS complexed to Cu(II) is also four-coordinate, with two sulfur ligands and two imidazoles. This would indicate that Cu(II), and possibly Cu(I), Co(II), and Zn(II), all bind to the same four ligands on InrS, which would then activate the conformational changes that lead to DNA release. Under normal cellular conditions the Zn(II) and Cu(I)/Cu(II) trafficking system would prevent InrS from binding to these metals which renders metal selectivity unnecessary.[1]

XAS on H21L-InrS complexed to Ni(II) in NaBr buffer was done to determine whether a loss of an imidazole ligand was visible and thus could allow for H21L to be assigned as the second imidazole ligand. The complex had a four-coordinate planar geometry, identical to WT-InrS complexed to Ni(II), but with non-overlapping XANES indicating that a change in coordination had occurred. EXAFS analysis gave a best fit with two S-donor ligands, one N/O-donor ligand and an imidazole from a histidine. This would thus indicate that H21 is a ligand, and loss of this ligand led to replacement by another protein residue or a water molecule. Unlike WT-InrS, the fit with two imidazole ligands is not significantly worse and is still considered a good fit (%R< 5). This may indicate that another imidazole ligand in the histidine rich N-terminus of InrS has replaced H21 in the coordination sphere. While the exact number of ligands cannot be

stated with confidence, this is a significant change from WT-InrS where the best fit consists of two imidazole ligands.

Based on the XAS analysis it is clear that InrS performs a similar function to RcnR through a different ligand set and geometry. However, because RcnR and InrS appear to have a different mechanism to ensure metal selectivity this difference in the first coordination sphere could be a byproduct of this difference. InrS is promiscuous and does not need to select for Ni(II) specifically, as the cellular complement of metal traffickers do not give it a choice of metal. RcnR is not promiscuous, and previous experiments indicate that the cellular trafficking components are not sufficient to keep non-cognate metals out of its metal site.[6,22] As InrS has the same W-X-Y-Z 'fingerprint' as some known promiscuous CsoRs, it could be that the fingerprint is not an indicator of cognate metal or geometry, but mechanism (see Chapter 4).

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CHAPTER 6

PREVENTION OF CELLULAR DAMAGE BY SUPEROXIDE

6.1 Generation and Effects of Superoxide

The mitochondrial free radical theory of ageing posits that reactive oxygen species (ROS) generated in the mitochondria is a consequence of aerobic respiration and is a primary cause of damage within the cell.[1–3] Over time damage that is not repaired accumulates, leading to breakdown of cellular machinery, age-related diseases and ageing. While most scientists agree that mitochondrial ROS are an important part of ageing, they agree that it is not the sole cause.[4–7] Because age is a primary risk factor in many diseases, understanding the role of ROS in disease can help develop therapies to relieve the burden of disease and allow an understanding of other factors involved in ageing.

Superoxide is primarily generated in the mitochondria and occurs when a single electron leaks during electron pair transport during oxidative ATP production.[3] There are seven accepted sites of electron leakage along the electron transport chain. Superoxide detoxification is performed by superoxide dismutases (SODs) of which there are three types; MnSOD, found in mitochondria of eukaryotes and bacteria, and FeSOD, found primarily in prokaryotes and chloroplasts; CuZnSOD, found in the cytosol and/or extracellular matrix of nearly all eukaryotes; and NiSOD found exclusively in prokaryotes. The absolute importance of superoxide levels outside the mitochondria are in debate, as neither CuZnSOD knockouts or antioxidant overexpression in mice have an effect on health or lifespan.[8–10] This is why many scientists consider ROS to be only one

factor in ageing. However, the importance of MnSOD in the mitochondria is not in debate, as MnSOD knockout studies in mice show this to be lethal, with mice surviving only 10-20 days although overexpression has not been conclusively linked to longevity.[11,12]

Oxidative stress caused by ROS such as superoxide has been strongly linked to atherosclerosis,[13,14] hypertension,[15–17] cancer,[1] diabetes,[18] Parkinson's,[19,20] and Alzheimer's[21,22] and has been implicated in many other diseases.[23–27] In addition to ageing, oxidative stress by smoking[28,29] and pollution[30–32] exacerbate these issues with pollution becoming a more prominent concern with many industrialized societies.

While the exact molecular mechanism of cellular damage by cigarette smoke is still not known primarily because of the debate of free radical lifetimes generated while smoking, it is undeniable that first and secondhand cigarette smoke causes and exacerbates many diseases. Cigarette tar is composed of a conjugated quinone polymer and is thought to produce high and stable levels of semiquinone radicals, which react with molecular oxygen to produce superoxide and is subsequently inhaled.[33] Because cigarette tar is stationary within the filter and the semiquinone radical is regenerated within the matrix there is a constant source of superoxide while smoking. Superoxide generation within cigarette smoke is less concrete primarily due to the short lived nature of radicals produced.[34,35] This has led to the steady state gas radical hypothesis, where the high level (300-500 ppm) of NO radicals present within cigarette smoke[36] react with nearby molecules on a continuous basis to form highly reactive NO_2 which further react with nearby molecules. In addition, tobacco is a highly complex mixture made of up over 3000 compounds, many of which are not ROS but which cause cellular damage and

dysfunction, leading to production of superoxide as a byproduct.[37] In particular, cigarette smoke is known to activate alveolar macrophages and produce high quantities of superoxide.[38]

In a similar vein to cigarette smoke, there is strong evidence suggesting that many of the compounds in air pollution are genotoxic, mutagenic, and carcinogenic.[30–32,39–41] Air pollution is characterized by a high production of ROS both extracellularly and within the mitochondria and activates alveolar macrophages which exhibit similar characteristics as smokers.[30–32,41] However, air pollution is a broad term that describes an extremely complex poorly defined mixture. Respirable particulate matter (PM) is a significant constituent of air pollution and is the primary health risk.[30,41] The composition of PM is diverse, but contains high levels of redox active heavy metals (Fe(III), Cu(II), Mn(II)), as well as carcinogenic polycyclic aromatic hydrocarbons.[31,40] PM in air pollution causes mitochondrial dysfunction and electron leakage, leading to high superoxide generation which causes damage to all cellular macromolecules and eventually to a variety of other diseases.[30–32,39–42]

Humans already have a mitochondrial superoxide dismutase (MnSOD) as well as a cytosolic and extracellular superoxide dismutase (CuZnSOD) and SODs are enzymatically perfect, with a diffusion limited k_{cat} of ~10^9 $M^{-1}s^{-1}$.[43] In order to combat the effects of excess superoxide generated by environmental factors (inflammation, pollution, ultraviolet rays, smoking, etc.) a superoxide mimic that will not interfere with biological functions or be recognized by our immune system is needed. Thus understanding how NiSOD, an exclusively prokaryotic SOD that is unique to the other SOD classes, functions will allow us to make NiSOD mimics that can be utilized *in vivo*

when needed. As humans contain no nickel requiring proteins, and the biochemistry that allows nickel to obtain a biologically accessible redox potential is highly specific, the mimic cannot be mismetalated or alternately metalated *in vivo* and would contain a relatively nontoxic metal (see section 1.2) that would not interfere with any native proteins.

6.2 Superoxide Dismutase

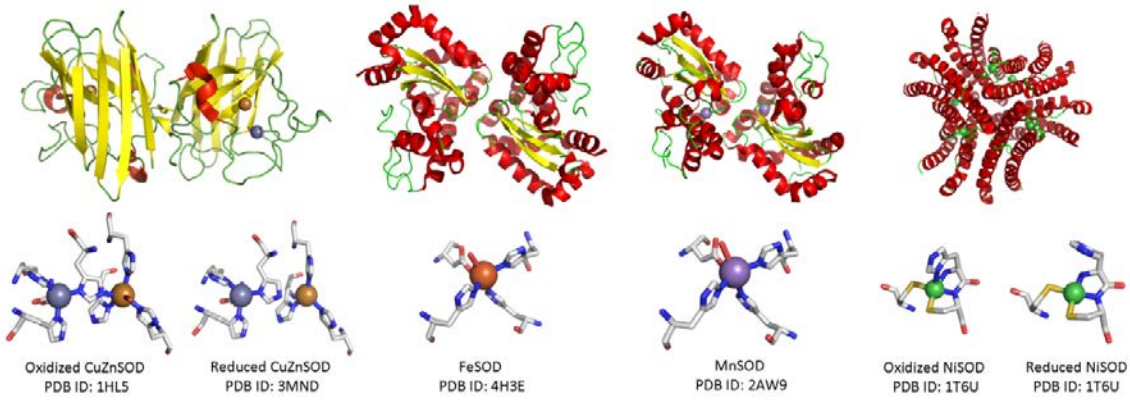

Figure 6.1: The quaternary structure and active site structures of Cu/Zn-, Fe-, Mn-, and NiSOD. The PDB ID used to generate the figure is indicated for each SOD. α-helices are shown in red, beta sheets in yellow and random coils in green.

There are three main classes of superoxide dismutases differentiated primarily by their active site metal, although FeSOD and MnSOD are typically grouped into the same class due to similar protein folds and active site composition despite being unable to functionally substitute metals although there are exceptions to this rule (**Figure 6.1 and 6.2**). These classes are CuZnSOD, Mn/FeSOD, and NiSOD. In addition to utilization of distinct metals, they are found in different domains of life, have different folds, amino acid sequences, active site composition, and mechanisms (**Figure 6.2**). Despite these

differences, all four SODs perform the same two half reactions (eq. 1-2) at the same diffusion limited rate (10^9 $M^{-1}s^{-1}$).

$$O_2^{\bullet -} + M^{Ox} \rightarrow O_2 + M^{Red} \quad (1)$$

$$O_2^{\bullet -} + 2H^+ + M^{Red} \rightarrow H_2O_2 + M^{Ox} \quad (2)$$

$$2\ O_2^{\bullet -} + 2H^+ \rightarrow O_2 + H_2O_2 \quad (3)$$

6.2.1 CuZnSOD

Activation of CuZnSOD is well studied and requires acetylation of the N-terminus, zinc and copper insertion, intrasubunit disulfide formation, and oligomerization.[44,45] Zinc insertion does not require a chaperone or disulfide bond formation.[46]

CuZnSOD exhibits diversity in its oligomeric state with eukaryotic intracellular CuZnSOD being dimeric and extracellular CuZnSOD being tetrameric. Bacteria typically contain CuZnSOD in the periplasm as a monomer or dimer. While the protein fold is conserved across species, the dimeric interfaces are different, accounting for this difference in oligomeric state. Human CuZnSOD (hCuZnSOD) is a dimer in all cases as long as the intersubunit disulfide bond is present.[47,48] Subunit interactions in yeast and bacteria are much weaker leading to readily exchangeable subunits.[49] Unlike MnSOD, CuZnSOD surface charge does not direct superoxide to the active site. Instead, superoxide guidance is performed primarily due to Arg143.[50] Mutation to neutral Ile reduces the rate constant by one order of magnitude while mutation to oppositely charged Asp or Glu reduces the rate constant by two orders of magnitude.[50,51] Protonation of the Asp or Glu residue increased the rate constant by one order of magnitude, comparable to the neutral Ile mutation.

While zinc insertion is relatively simple,[52] copper insertion may or may not require the copper chaperone for SOD1 (CCS) depending on the organism.[53,54] In addition to copper insertion, CCS can promote intrasubunit disulfide formation in an oxygen dependent manner, but is not absolutely required for either event to occur.[45] Both yeast and humans can produce small quantities of active CuZnSOD in the absence of CCS.[53] Bacteria and *C. elegans* have been shown to completely oxidize and metallate CuZnSOD without CCS.[54] Part of this is due to the fact that the reduction potential of the disulfide bond is organism dependent and in some organisms there exists a second pathway in which copper is delivered and inserted by glutathione and the disulfide bond is formed in an oxygen independent manner.[55] CCS can be divided into three domains with Domain I containing an MXCXXC copper binding motif which has been shown to deliver copper to SOD1.[56] Domain II is a CuZnSOD homolog and allows for dimerization to allow for copper insertion and disulfide bond formation.[56] Domain III contains a CXC motif and evidence suggests it may be involved in disulfide bond formation.[56]

The structure of the copper center in the binunclear active site is dependent on the oxidation state of the copper center (**Figure 6.1**). In either state, the active site zinc ion is ligated by His63, His71, His80, and Asp83 in a tetrahedral geometry.[57] In the reduced form (Cu(I)) the copper is ligated by His46, His48, and His120 in a trigonal planar geometry.[57] Upon oxidation to Cu(II), the His63 bound to the zinc deprotonates and binds to Cu(II) along with a water molecule resulting in a 5-coordinate square-pyramidal geometry.[43,57] The forward reaction (equation 1 above) proceeds in a pH- and Zn-independent manner with a rate constant of 10^9 $M^{-1}s^{-1}$.[46] The reverse reaction (equation 2

above) is pH dependent at a pH > 6 when zinc is absent.[58] This is because the protonated His63 in the reduced state bound to zinc is the source of one of the protons and without a second metal is not in a catalytically relevant position. In addition, without a second metal, the copper ion can occupy this position which is catalytically inactive.

The functional importance of CuZnSOD is organism dependent. In yeast, ΔCuZnSOD leads to a variety of growth defects that can be traced back to high oxidative damage, such as auxotrophy for lysine, leucine, and methionine.[59,60] The first two are due to superoxide attack on [FeS]-cluster containing proteins within the metabolic pathway.[59] Methionine auxotrophy has been traced to oxidative depletion of NADPH, required in the methionine biosynthetic pathway.[60] In *Drosophilia* ΔCuZnSOD leads to infertility and an 80% reduction in lifespan.[61] In female mice, ΔCuZnSOD causes infertility[62] in addition to accelerated age related muscle atrophy,[63] hearing loss,[64] and eye diseases[65] in all mice. In addition, a recent experiment revealed that while ΔCuZnSOD from one parent does not affect lifespan in mice, an inherited deletion from both parents reduces lifespan by ~30%.[66] However, in bacteria and *C. elegans,* deletion of CuZnSOD has no observable health effects.[8] *C. elegans* has five SOD genes, and deletion of all five does not result in any effects other than slightly higher oxidative stress.

6.2.2 FeSOD

FeSOD is considered to be in the same enzyme class as MnSOD because of their similar protein folds and identical first coordination sphere (**Figure 6.2**). Despite their structural similarities the metal ions are not catalytically interchangeable, with a Mn in FeSOD resulting in slow disproportionation and vice versa.[67] This has been attributed to

differences in their innate redox potentials which requires different protein environments in order to tune it to a catalytically relevant potential.[68–71]

The active site iron is coordinated in a trigonal bipyramidal geometry by His26, His73, His160, Asp156, and one H_2O/OH^- (*E. coli* FeSOD numbering, **Figure 6.2**). Similar to MnSOD, when performing the forward reaction (equation 1 above) the bound ligand is a hydroxide which obtains a proton during oxidation of superoxide to generate a water ligand.[43,72] This proton is then donated to superoxide during reduction to H_2O_2.[43,72] This proton is regenerated from bulk solvent via a hydrogen bonding network that also stabilizes the water ligand.[70]

In the reaction pertaining to Equation 1 superoxide is thought to bind directly to Fe(III) to allow for electron transfer. This is in contrast to MnSOD, where superoxide binding leads to an inhibited complex.[73–77] Small anion binding to the Fe(III) state of FeSOD has been shown for N_3^-, F^-, and OH^-.[78–80] At high pH the k_{cat} remains the same while the K_M decreases, which is consistent with OH^- as an inhibitor.[70,81] Tyr34 acts as a small anion selectivity filter, as the K_D is lower for small anions in WT FeSOD and higher in the Y34F mutation and excludes anions larger than superoxide.[82] These larger

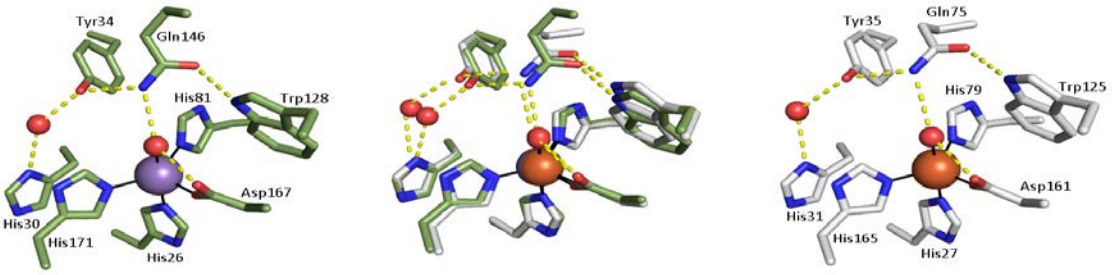

Figure 6.2: Active site representations of Mn-SOD (Left, PDB ID 1D5N) and Fe-SOD (Right, PDB ID 1MY6), with the two structures overlaid (Center). Waters are shown as red spheres, with hydrogen bonds depicted as yellow dotted lines.

anions do act as competitive inhibitors but more likely by blocking access to the Fe(III) center and not by direct binding.

In contrast, in the reverse reaction superoxide does not bind to Fe(II) but forms hydrogen bonds with the Fe(II) bound water molecule and Tyr34.[83] This is most likely because if superoxide can bind, then so can the peroxide anion HO_2^-, which can interact with Fe(II) and perform Fenton chemistry.[84] Experiments on NMR titrations with F^- reveal backbone shifts at and near Tyr34 but not the catalytic Fe(II) center.[82,85] Current theory based on computations proposes that the water ligand donates a proton to the proximal oxygen of superoxide and the distal oxygen engages in a hydrogen bond with Tyr34.[86] This allows Tyr34 to donate a second hydrogen which is replenished by solvent, as Tyr34 is involved in the hydrogen relay that also protonates the Fe(II) bound water molecule. The k_{cat} has a solvent isotope effect that signifies this protonation step involves a solvent exchangeable proton[70] and acidic buffers only have a weak acceleration effect,[87] indicating an internal proton transfer. Because K_M increases at basic pH values but k_{cat} does not, this donor must be protonated up to a pH of 11. Both Tyr34 and the water ligand meet these criteria. Calculations indicate that if the water ligand donates a proton to the distal oxygen of superoxide it would become stably bound to the Fe(II) center and is not in a position to accept a second proton from Tyr34.[86]

6.2.3 MnSOD

MnSOD is found in the cytosol of prokaryotes, and has been found in the mitochondria and cytosol of eukaryotes as well as in chloroplasts.[43] The importance of MnSOD depends on its location and the environment of the organism. MnSOD present in mitochondria is of critical importance, as shown by mouse studies where MnSOD was

deleted, which lead to a 10-20 day lifespan.[11,12] Deletion of CuZnSOD located in the cytosol of mice is not lethal nor does it show a reduction in lifespan.[62,88]

There is currently no identified chaperone for MnSOD in any organism despite MnSOD being specifically metalated in all organisms even in the presence of high levels of iron, which *in vitro* has almost identical affinity.[89] Recently a gene, Mtm1, was identified as a mitochondrial Mn transporter but Δmtm1 retained high intra-mitochondrial levels of Mn as compared to WT, but had low levels of incorporation into apo-MnSOD indicating a role in metal insertion.[90,91] Metalation was found to be a temperature dependent process, occurring only at physiologically relevant temperatures (i.e. not at standard laboratory experiment temperatures between 20-25 ^{o}C) and which leads to nonspecific metalation *in vitro*.[92,93] Unlike CuZnSOD there is no structural difference between apo- and holo-MnSOD indicating a structural destabilization during metal entry or a switch between two states that occurs at physiological temperatures.[94,95] If there is a specific chaperone for insertion, as the lack of mismetalated MnSOD suggests, the chaperone likely imparts instability or biases the protein toward the conformation that allows for metal insertion.

MnSOD is found as a dimer in prokaryotes and a tetramer in eukaryotes. Oligomeric state does not affect mechanism or rate constant, but tetrameric MnSOD does have increased resistance to heat, pH, and denaturant induced unfolding.[96] In addition all MnSOD have a surface charge that electrostatically guides superoxide to the active site channel.[97] For all MnSOD across all species the active site consists of three His residues, 1 Asp residues and a water/hydroxide ligand arranged in a trigonal bipyramidal geometry which is the same in both the oxidized and reduced state (**Figure 6.1** and **6.2**).

The MnSOD is mechanistically unlike the other SODs due to it having distinct activities when exposed to high or low concentrations of superoxide. This is a phenomenon called 'gating' which occurs at high concentrations of superoxide relative to the enzyme and causes superoxide disproportionation in a biphasic process comprised of a fast and slow step.[74–77] The fast step is the standard ping pong mechanism detailed in equations 1 and 2 and thought to proceed by an almost identical mechanism as FeSOD as detailed above. The slow step is an inhibition complex that is thought to be comprised of superoxide binding directly to the Mn center.[74–77] The amount of time and concentration dependence of this inhibited complex is dependent on the organism, with human mitochondrial MnSOD spending the most time in this complex.[73,98] Human mitochondria have recently been shown to generate large bursts of superoxide where MnSOD is inhibited, leading to a buildup of superoxide and a relatively steady state of H_2O_2.[99,100] This is related to H_2O_2 being a signaling molecule because a constitutively active SOD would generate high levels of H_2O_2 which would interfere with its role as a signaling molecule.

6.3 Nickel Redox Chemistry

The last family of SODs is comprised of NiSOD which is distinct from the other families in a variety of ways but the use of nickel as a redox active metal is the most unusual. In order to perform both half reactions the redox potential of the active site metal should ideally be right in the middle of the two half reactions (Eqns 1 and 2 above), 0.36 V.[101] Both iron and copper can dismutate superoxide in the absence of the protein environment (although their redox potentials do not allow for both half reactions).

Manganese in aqueous media cannot disproportionate superoxide[102] (with a redox potential of 1.51 V v. NHE[103]) but its redox potential can be tuned with a mixture of unreactive N/O ligands. This is not true of nickel, whose redox potential (2.26 V v. NHE[104]) in aqueous media is higher than that of manganese and cannot be tuned to a redox potential capable of performing both half reactions by just N/O ligands with 0.79 V v. NHE[105] being the lowest it can go. This redox potential is comparable to iron in aqueous media[103] and thus is capable of performing one half of the ping pong mechanism, the disproportionation of superoxide to oxygen.[43] In order to achieve a redox potential that can perform both half reactions, a ligand set that includes something beyond N/O ligands is needed. NiSOD achieves this by ligating the side chains of two cysteine ligands, both of which are needed in order to tune the redox potential appropriately.

Utilizing sulfur ligands in the active site is only a viable strategy provided you can prevent oxidation of the cysteine ligands which is difficult when the substrate is superoxide. This can be achieved through a variety of strategies; tune the electronic structure of the thiolate to make it more difficult to oxidize; alter the Ni(III) center to make it less oxidizing; or make it sterically impossible to form a disulfide. Proteins can easily perform the prevention of disulfide formation through sterics (although this is not the case in NiSOD). In addition, proteins are known to modify the potentials of ligands and metals within an active site pocket through surrounding hydrophobic or H-bond interactions. This can even be seen in the case of MnSOD which has the same first coordination sphere as FeSOD but whose redox potential must be tuned to a greater extent than iron in order perform both half-reactions.[43] However, the use of cysteine

thiolates to tune redox potential is not unique to NiSOD. Thiolate ligation can be seen in all known redox-active nickel enzymes ([NiFe]-hydrogenase, NiSOD, carbon monoxide dehydrogenase (CODH), acetyl-coenzyme A synthase (ACS)).[106] Recently two new nickel requiring enzymes have been discovered, lactate racemase, LarA,[107,108] and quercetinase, QueD.[106] However the structures and mechanisms of both of these proteins are currently unknown so whether they are redox active or follow the current trend of thiolate ligation is still unknown.

6.4 Nickel Superoxide Dismutase

6.4.1 NiSOD Structure

All currently characterized NiSODs are all α-helical hexamers (**Figure 6.1**). The oligomeric state of NiSOD is in contrast to the other SODs, none of which have been isolated as a hexamer and which have different oligomeric states depending on the organism (eukaryotic v. prokaryotic) or location in the organism (extracellular v. intracellular) (see section 4.2.1 – 4.2.3). In a similar manner to CuZnSOD, the active site structure of NiSOD differs depending on the oxidation state of the nickel center.[109] In the reduced state the Ni(II) is coordinated by the side chains of Cys2 and Cys6 as well the N-terminal amine and the backbone amide of Cys2 in a four-coordinate planar geometry (**Figure 6.1**). Upon oxidation to Ni(III) the side chain of His1 coordinates in an axial position resulting in a four-coordinate pyramidal geometry. While the axially bound histidine is observed in X-ray absorption spectroscopy,[110] X-ray crystallography,[109] and hyperfine splitting in EPR[111] its theoretical significance is up for debate as the movement

on and off the nickel center would be too slow to allow for a catalytic rate constant on the order of ~10^9 $M^{-1}s^{-1}$.

6.4.2 NiSOD Catalytic Mechanism

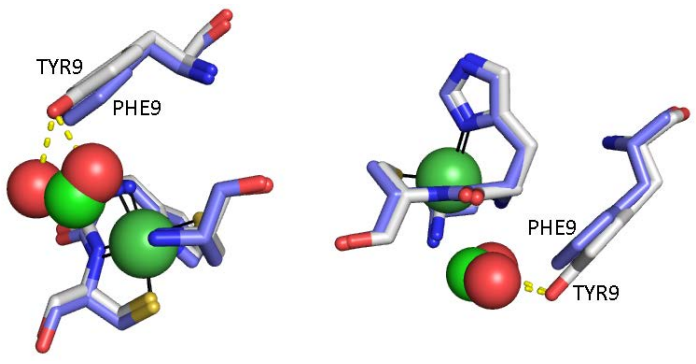

Figure 6.3: Active site overlay of WT-NiSOD (shown as white residues, PDB ID 1T6U) and Y9F-NiSOD (shown as blue residues, PDB ID 3G4X). Water molecules shown as red spheres, nickel ions as dark green, and the chloride ion shown as neon green sphere).

One of the main questions regarding NiSOD is whether it proceeds by an inner- or outer-sphere mechanism, or both like FeSOD. This question has not been answered and is currently a debate between experimental data, which argues for outer-sphere,[112,113] and theoretical calculations,[113] which argues for inner-sphere. Experimental data consists primarily of studies with azide which does not bind to the nickel center[112,113] but instead seems to bind in a similar position (interacting with Tyr9) as the chloride seen in the Tyr9Phe crystal structure[114] (**Figure 6.3)**. Tyr9 is thought to act in a similar manner to the Tyr34 in Fe/MnSOD, positioning the substrate and acting as a gateway to filter out larger ions. In the Asp3Ala mutation Tyr9 is shifted closer to the nickel center by 1 Å, and this mutant is irreversibly inhibited by H_2O_2, thought to be due to Tyr9 being unable to adequately position substrate and small anions away from the nickel center, supporting an outer-sphere mechanism.[114] However, this data on Tyr9 does not necessarily support

either an inner- or outer-sphere mechanism, as FeSOD utilizes Tyr34 in an almost identical manner and is thought to engage in a different mechanism for each half reaction.

The second half reaction involving reduction of superoxide and generation of H_2O_2 requires two protons in order to proceed. Like all SODs, NiSOD is pH independent at physiological pH values so the protons must come from the protein.[111] However, the location of the protons has not been definitively deduced. Theoretical calculations indicate that both protons come from Cys2 in two sequential protonations.[115,116] S K-edge XAS on H_2O_2 reduced NiSOD revealed a disappearance of pre-edge features corresponding to thiolate ligands, indicating both cysteines are protonated, in contrast to the theoretical studies.[117] However, WT NiSOD is reversibly inhibited by H_2O_2, and the S K-edge data revealed that H_2O_2 reduced NiSOD is structurally different than photoreduced NiSOD and reduction by peroxide is not a standard part of the ping-pong mechanism.[117] Studies on peptide maquettes utilizing the first 12 residues of NiSOD also support the donation of at least one proton from one of the cysteine residues, although this study proposed that the proton came from Cys6.[118,119]

6.4.3 Ni(III) Character

One mechanistically frustrating aspect of NiSOD is that it is isolated as 50% Ni(II) and 50% Ni(III) as determined by EPR integration.[111] NiSOD can be fully reduced although even this is tricky, as dithionite reacts with superoxide itself, and NiSOD is inhibited by H_2O_2. Metal based inhibitors could interfere with pulse radiolysis, as superoxide disappearance is monitored at 260 nm. However, these reactions can be compared to the other SODs, as they can all be fully reduced in the same manner. Unfortunately, NiSOD cannot be fully oxidized.[110,111,114] Regardless of the oxidant used,

NiSOD remains only 50% Ni(III) and thus cannot be studied from the position of the reverse reaction, Ni(III) → Ni(II). As a square-pyramidal species, the Ni(III) is a S = ½ center with a single unpaired electron in the d_{z2} orbital. In EPR it appears as an axially distorted rhombic species[111] (a rhombic species indicates that $g_x \neq g_y \neq g_z$ which makes sense given the structure of the nickel center).[120] The inability to fully oxidize NiSOD, despite its identical average structure by crystallography coupled with the ability of at least 3 of the nickel centers in the hexamer being Ni(III), is indicative of a protein mediated effect. This hypothesis assumes that the integration of the Ni(III) signal in EPR represents half the nickel centers in a single hexamer, and not half the hexamers in a sample.

6.5 Overview and Significance

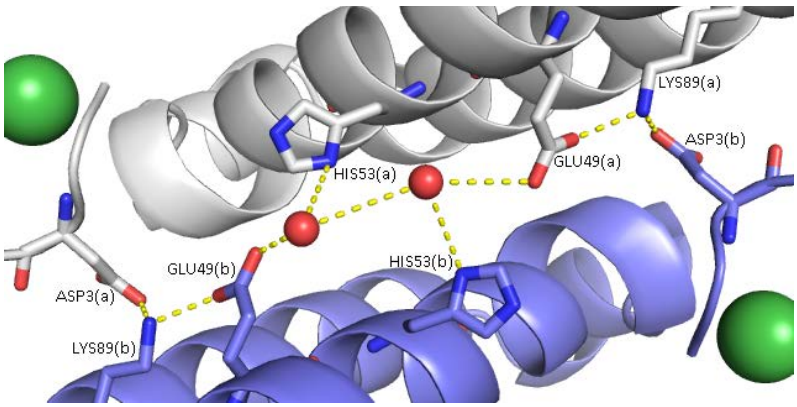

Figure 6.4: Ribbon diagram of dimer interface in WT-NiSOD (PDB ID 1T6U) with each monomer shown in a different color. Water molecules shown as red spheres, nickel ions shown as green spheres, and hydrogen bonds shown as yellow dotted lines.

The purpose of this thesis is to investigate the feature in NiSOD that prevents 100% oxidation to Ni(III). Each nickel site is 'connected' to another site via a complex hydrogen bonding network that has a twofold axis of symmetry and involves Asp3

bonding to Lys89, Glu49, and His53 (**Figure 6.4**). His53 is engaged in a water-mediated hydrogen bond with the symmetrically placed His53 from the adjacent monomer. This His53 is then bonded to Glu49, Lys89, and finally Asp3. These two nickel centers are 23 Å apart. If this hydrogen bonding network is indeed allowing communication, 100% oxidation should be achievable. This will allow us to study the mechanism of NiSOD starting from only the Ni(III) oxidation state, so the results will not be confused by the other half of the ping-pong mechanism. In addition, it might give us insight into why the protein prevents full oxidation.

6.6 References

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CHAPTER 7

DISRUPTION OF CROSSTALK BETWEEN NICKEL CENTERS IN NISOD

7.1 Introduction

NiSOD is the newest member of the SOD family of enzymes and is not comparable with the other SODs in amino acid sequence, secondary/quaternary structure, or in its active site structure and composition. These differences may be attributed to having an unconventional metal like nickel as the redox active metal center, thus structural elements would significantly differ from the other SODs containing more conventional active site metals. There is, however, one unusual feature of NiSOD that cannot be easily explained by its redox active metal center. Full oxidation of the redox active metal centers has been seen in CuZn, Fe, and MnSOD, and in the case of MnSOD,

Table 7.1: Amount of Ni(III) and k_{cat} in all currently studied NiSOD mutants.

NiSOD	% Ni(III)	K_{cat} (M^{-1} s^{-1})
WT[1]	51	5.3×10^9
Recombinant WT[2]	51	7.07×10^8
D3A[2]	48	2.09×10^8
Y9F[2]	53	3.71×10^8
Y62F[2]	48	6.42×10^8
Y9F/Y62F[2]	46	2.41×10^8
H1A[3]	0	4.7×10^7
Ala0[4]	0	1×10^6
C2S[5]	0	5.0×10^6
C6S[5]	0	3×10^6
C2S/C6S[5]	0	1×10^6
R47A[3]	15	1.21×10^8
E17A/R47A[3]	0	3.6×10^7
E17R/R47E[3]	8	9.5×10^7
H1*[6]	11	5.6×10^6

full oxidation occurs naturally in air.[7] It has been previously reported that WT-NiSOD is isolated as 50% Ni(II) and 50% Ni(III) and even under oxidizing conditions this ratio is unaltered.[1,2] In all currently studied mutants of NiSOD, there has never been an observed increase in the amount of Ni(III), only a decrease (**Table 7.1**), indicating that it is quite easy to destabilize the Ni(III) species. If the oxidation state of the nickel is changing during reaction, then this suggests that all the nickel centers are capable of being oxidized to Ni(III). The most logical explanation is that there is internal cross-talk preventing full oxidation, presumably between two adjacent monomers, which would explain the ratio of Ni(II) to Ni(III) in as-isolated or oxidized samples.

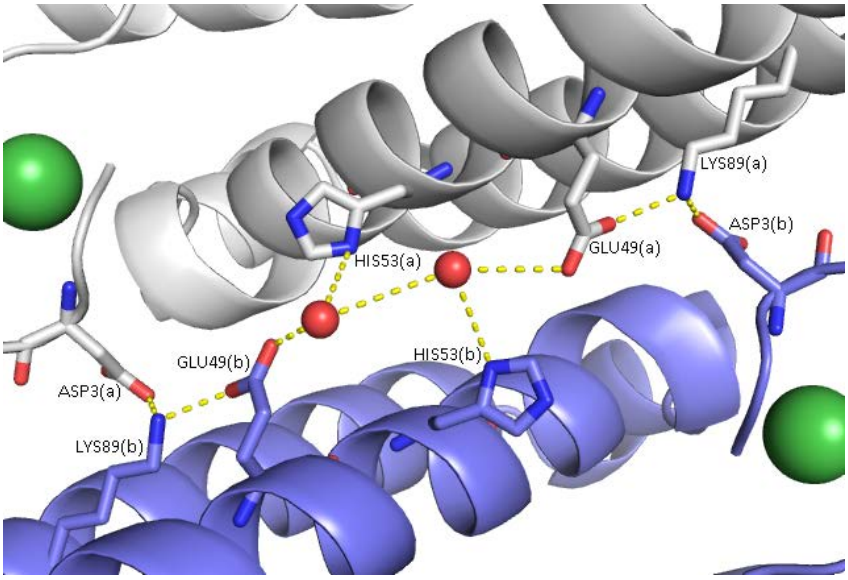

Figure 7.1: Ribbon diagram of the symmetrical hydrogen bonding network connecting two nickel centers in WT-NiSOD (PDB ID 1T6U) with each monomer shown in a different color. Water molecules shown as red spheres, nickel ions shown as green spheres, and hydrogen bonds shown as yellow dotted lines.

Analysis of the crystal structure of WT-NiSOD reveals a hydrogen bonding network with a twofold axis of symmetry connecting two adjacent metal centers (**Figure**

7.1). This bonding network involves Asp3, Lys89, Glu49, and His53, with the His53 from one monomer engaged in a water-mediated hydrogen bond with His53 from the adjacent monomer. Because NiSOD is a homo-hexamer, each monomer is identical.

The goal of the work presented in this chapter is to test the role of the symmetrical hydrogen bonding pathway that allows the redox status of one metal site to influence the other site. This was accomplished by mutation of the central His53 residue in the aforementioned network, which might break the communication between nickel sites and allow full oxidation of NiSOD. Direct observation of the structural changes that occur at the metal center will be accomplished with X-ray absorption spectroscopy (XAS), which will give information on coordination number, ligand type and bond distances. EPR will be used to determine the oxidation state of the enzyme and quantify the amount of Ni(III) present after oxidation. To assess the effect of this "redox cooperativity" on the activity of the enzyme, kinetic studies of the catalytic reaction rate were undertaken using pulse radiolytic generation of O_2^- and monitoring the rate of disappearance of O_2^- via its absorbance at 260 nm. The effects of these mutations on the quaternary structure will be monitored by size exclusion chromatography. Finally, changes in the electronic properties of the enzyme will be assessed by UV-Vis spectroscopy.

7.2 Experimental Procedures

7.2.1 Cloning and Mutagenesis

The NiSOD gene from *Streptomyces coelicolor* with a pelB leader sequence was synthesized and inserted into pET-22b by GENEWIZ, Inc. The H53A point mutation was then introduced into the NiSOD gene on the pET-22b vector using the QuikChange

(Stratagene) site-directed mutagenesis method. The mutation was made using the primers 5'-CGCGCCGAGCTCGCGAAGGCCCACGTCTCCGTGC-3' and 5'-CCACAGCACGGAGACGTGGTGCTTCGCGAGC-3'. The PCR product was directly transformed into NovaBlue (Novagen) competent cells and plasmids that were re-isolated from transformants on a plate containing ampicillin at 100 μg/mL. The presence of the desired mutation was confirmed in each case via sequencing at GENEWIZ Inc. (South Plainfield, NJ).

The NiSOD gene with the H53A mutation was then cloned out of the pET-22b-sodN vector using the PCR amplification primers 5'-GAGGCTCACAGAGAACAGACCGGTGGTCACTGCGACCTGCCTTGC-3' and 5'-CTCAGTGGTGGTGGTGGTGGTGCTCGAGTTAGGCCTTCTTGGTCTCCC-3'. The PCR product was purified from a 1% agarose gel and inserted into pET23SUMO[8] using the Gibson assembly method.[9] The PCR product was transformed into NovaBlue (Novagen) competent cells and plasmids were re-isolated from transformants on a plate containing ampicillin at 100μg/mL. Successful insertion of the H53A-NiSOD gene into pET-23SUMO was confirmed via sequencing at GENEWIZ Inc. (South Plainfield, NJ).

7.2.2 NiSOD Expression and Purification

Distinct expression and purification strategies were developed for pelB-WTNiSOD and SUMO-H53ANiSOD fusion proteins. For the pelB-WTNiSOD construct, pelB-WTNiSOD was transformed into DL41 (DE3) cells. A single colony of *E. coli* DL41 (DE3) with the plasmid encoding the NiSOD protein was grown overnight at 37 °C in a Luria-Bertani broth (LB) culture, supplemented with ampicillin (amp) at 100 μg/mL. An aliquot (10 mL) of the overnight culture was added to 1 L of fresh LB with amp

added. The cultures were incubated at 37 °C with shaking until an OD_{600} of ~0.8 was reached and then induced by addition of β-D-1-thiogalactopyranoside (IPTG) (CarboSynth) to a final concentration of 0.8 mM. The cultures were then incubated with shaking for an additional three hours. The cultures were pelleted at 4000 g for 15 minutes and then gently resuspended in 100 mL of osmotic shock buffer (20% sucrose, 1 mM EDTA, 30 mM Tris HCl, pH 8.0) per liter of culture. The resuspended cells were shaken at 180 rpm for 15-20 minutes at room temperature and then centrifuged at 4000g for 10 minutes. The supernatant was discarded and the cells were gently resuspended in 100 mL of ice cold 5mM $MgSO_4$ per liter of culture. The resuspended cells were shaken at 4 ^oC for 10 minutes and then centrifuged at 10,000g for 10 minutes. The pellet was discarded and the supernatant was collected for further purification.

Chromatographic purification of WT-NiSOD employed an AKTA-FPLC system (Amersham Biosciences) and a peristaltic pump (Gilson). The supernatant was loaded onto a hand packed 5 mL QSepharose FF column. The column was washed with buffer A (50 mM Tris, pH 8.0) and then eluted in one step with buffer B (50 mM Tris, 1 M NaCl, pH 8.0). The fraction containing WT-NiSOD as determined by SDS-PAGE was then loaded on a 120 mL HiLoad 16/60 Superdex 75 (GE Life Sciences) column equilibrated with buffer C (50 mM Tris, 200 mM NaCl, pH 8.0). Fractions were collected on the basis of absorbance at 280 nm. An SDS-PAGE gel was run to determine which fractions contained WT-NiSOD.

SUMO-H53ANiSOD was transformed into *E. coli* BL21 (DE3) pLysS cells. A single colony of *E. coli* BL21 (DE3) with the plasmid encoding the NiSOD protein was grown overnight at 37 °C in a Luria-Bertani (LB) broth culture supplemented with

ampicillin at 100 μg/mL. An aliquot (10 mL) of the overnight culture was added to 1 L of fresh LB culture with ampicillin added. The cultures were incubated at 37 °C with shaking until an OD_{600} of ~0.8 was reached and then induced by addition of β-D-1-thiogalactopyranoside (IPTG) (CarboSynth) to a final concentration of 0.8 mM. The cultures were then incubated with shaking for an additional three hours. The cells were harvested by centrifugation at 5500g, resuspended in residual media and frozen at -80 °C. The lysed cells were thawed in a 37 °C water bath, and each liter of culture was treated with 20 μL DNase I solution (10 mg/mL DNase I, 40% glycerol), 45 μL of 1 M tris(2-carboxyethyl)-phosphine hydrochloride (TCEP) (Soltech Ventures), and 65 μL of 200 mM phenylmethyl-sulfonylfluoride (PMSF) (MP Biomedicals). The lysed cells were then incubated at 37 °C for 45 minutes. The cell lysate was centrifuged at 15000 g and the supernatant was used for protein purification.

Chromatographic purification of SUMO-H53ANiSOD employed an AKTA-FPLC system (Amersham Biosciences) and a peristaltic pump (Gilson). The lysate was loaded onto a 5 mL hand packed NiNTA HisBind Superflow (Novagen) column and washed with NiNTA binding buffer (100 mM Imidazole, 50 mM Tris, 300 mM NaCl, pH 8.0). The column was washed with 12% elution buffer (500 mM Imidazole, 50 mM Tris, 300 mM NaCl, pH 8.0) before the fusion protein was eluted with 100% elution buffer. The SUMO-tagged protein was cleaved by the Ulp-His protease.[10] The mixture was loaded onto a hand packed Butyl Sepharose FF (GE Life Sciences) and washed with Butyl binding buffer (50 mM Sodium Phosphate, 2 M NH_4SO_4, pH 8.0) and then washed with 40% Butyl Elution Buffer (50 mM Sodium Phosphate, pH 8.0). H53A-NiSOD was eluted with 60% Butyl Elution Buffer. The fractions containing H53A-NiSOD as

confirmed by SDS-PAGE were run over a MonoQ 5/50 GL (GE Life Sciences) and washed with buffer A (50 mM Tris, pH 8.0) followed by a linear gradient of 0 to 100% buffer B (50 mM Tris, 1 M NaCl, pH 8.0) over 25 mL at a flow rate of 1.5 mL/min while 0.5 mL fractions were collected. Fractions containing H53A-NiSOD (in red box shown below) were determined by SDS-PAGE and used without further purification.

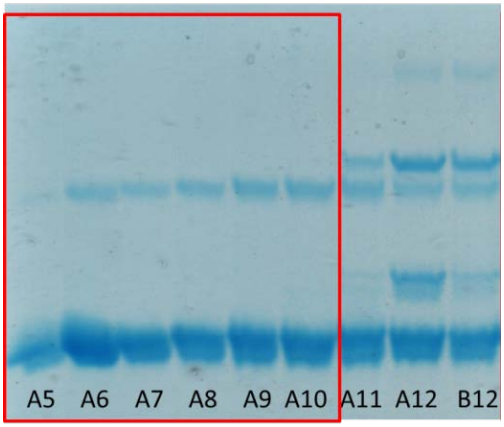

Figure 7.2: SDS-PAGE gel of a MonoQ column. Gels pooled for further use boxed in red.

The expected molecular weights of the purified proteins were confirmed using electrospray ionization mass spectrometry (ESI-MS) using an ABI-SCIEX QSTAR-XL equipped with a turbo-spray ESI source in sequence with an Agilent 1100 HPLC system with a BioBasic-8 (Thermo Scientific) column for salt removal. The molecular weights of WT- and H53A- NiSOD were calculated as 13200.96 Da, found: 13199.11 Da, calculated: 13134.90 Da; found: 13132.4 Da.

7.2.3 Metallation of NiSOD

The processed protein was reduced with a 5-fold excess of tris(2-carboxyethyl)-phosphine hydrochloride (TCEP) (Soltech Ventures) and reconstituted with a 3-fold excess of $NiCl_2$ in an anaerobic glovebox (Coy Laboratory Products, Inc.). Excess TCEP and Ni were removed by concentrating with a microspin concentrator (Millipore, 3 kDa

MWCO). A PerkinElmer Optima 4300 DV inductively coupled plasma-optical emission spectrometer was used to quantify the nickel content of the reconstituted mutant proteins. The sample introduction system consisted of a concentric nebulizer with a cyclonic spray chamber. The concentration of nickel in each sample was determined at a λ of 231.604 nm.

7.2.4 Size Exclusion Chromatography

Size-exclusion chromatography was performed using a Superdex 75 15/300 GL (GE Healthcare) column. The column was standardized with the Gel Filtration Standard (Bio Rad). A standard curve was constructed by plotting V_e/V_0 versus the molecular mass (where V_e is the elution volume of the peak, and V_0 is the elution volume of thyroglobulin), and the data were fit with an exponential decay. All proteins were injected onto the column at a concentration of 100 μM (monomer) in 50 mM Tris, 100 mM NaCl pH 8.0, and the retention volumes of the peak(s) (V_e/V_0) from each chromatogram were analyzed using the standard curve to determine the molecular weights of the eluted proteins.

7.2.5 Differential Scanning Calorimetry

DSC thermograms were measured with a DSC-Q200 (TA Instruments, Inc.). NiSOD samples were concentrated to 300 μM in 20 mM Tris (pH 8.0), 150 mM NaCl and loaded and hermetically sealed in sample pans. Spectra were collected between 30 to 100 °C at a scan rate of 1 °C/min. Baseline correction and normalization were performed with the Origin graphing program. Peak maxima were taken as melting temperatures, T_m.

7.2.6 Kinetics

The pulse radiolysis experiments were carried out using a 2-meV Van de Graaff accelerator at Brookhaven National Laboratory in collaboration with Dr. Diane Cabelli. Superoxide radicals were generated upon pulse radiolysis of an aqueous, air/O_2-saturated solution containing 10 mM phosphate, 30 mM formate, and 5 μM EDTA (Eqs. 6–10):

$$OH + HCO_2^- \rightarrow H_2O + CO_2^- \quad (6)$$

$$CO_2^- + O_2 \rightarrow CO_2 + O_2^- \quad (7)$$

$$e_{aq}^- + O_2 \rightarrow O_2^- \quad (8)$$

$$H + O_2 \rightarrow HO_2 \quad (9)$$

$$HO_2 \rightarrow O_2^- + H^+ \quad (10)$$

Catalytic rate constants were obtained by monitoring the disappearance of O_2^- at 260 nm in the presence of micromolar concentrations of NiSOD. The path length of the quartz cell used was 2.0 cm and a 100 – 700 ns pulse width was chosen, resulting in the generation of 1 – 7 μM O_2^- per pulse. The reported rate constants are based on metal concentration, with the assumption that all nickel ions are specifically bound and contribute equally to O_2^- dismutation.

7.2.7 UV-Vis Spectroscopy

Spectra were recorded under anaerobic conditions on a Hewlett-Packard 8453 UV-visible spectrophotometer. Metallated NiSOD was diluted in 50 mM Tris, 100 mM NaCl, pH 8.0 to a final concentration of 100 μM in gas-tight quartz cuvettes (FireflySci). Two molar equivalents of dithionite were added for reduction of NiSOD and two molar equivalents of $IrCl_6$ were added for oxidation of NiSOD in an anaerobic glove bag (Coy Laboratory Products, Inc.) and mixed by inversion.

7.2.8 Electron Paramagnetic Resonance (EPR)

Experiments were performed on 200 μL samples containing WT- or H53A-NiSOD (500 μM based on nickel concentration) in 20 mM Tris, 100 mM NaCl, pH 8.0. For the reduction of NiSOD two molar equivalents of dithionite were added in an anaerobic glove bag (Coy Laboratory Products, Inc.). The oxidized sample was prepared by adding two molar equivalents of $K_3[Fe(CN)_6]$. The samples were allowed to incubate for an additional 5 minutes at 23°C, at which point they were transferred to EPR tubes and flash frozen in liquid nitrogen. EPR samples were run using a finger dewar on a Bruker Elexsys E-500 EPR equipped with a DM4116 cavity at 9.609 GHz frequency, 6.0 131 mW power, 10G modulation amplitude, 100 GHz modulation frequency, 327 ms time constant, 77K.

7.2.9 X-ray Absorption Spectroscopy

Samples of the metallated proteins were concentrated to ~1-4 mM metal and a total volume of ~50 μL in buffer containing 50 mM Tris, 100 mM NaCl, 10% glycerol, pH8.0 using microspin concentrators (Millipore). The concentrated samples were injected into polycarbonate XAS sample holders wrapped in kapton tape, and then rapidly frozen in liquid nitrogen and stored at -80 ^{o}C.

XAS data collection for all complexes of WT- and H53A-NiSOD bound to Ni(II) were collected at the Stanford Synchrotron Radiation Laboratory (SSRL) on beam line 9-3. The samples were cooled to ~10 K using a liquid helium cryostat (Oxford Instruments) and the ring conditions were 3 GeV and 450-500 mA. Beam line optics included a Si(220) double-crystal monochromator. X-ray fluorescence data was collected using a 100-element detector (Canberra). A Soller slit with a Z-1 element filter was placed between the sample chamber and the detector to minimize scattering.

Internal energy calibration was performed by collecting spectra simultaneously in transmission mode on the corresponding metal foil to determine the first inflection point on the edge, which was set to 8331.6 eV for Ni. X-ray absorption near-edge structure (XANES) data were collected from -200 to +200 eV relative to the metal K-edge. Extended X-ray absorption fine structure (EXAFS) data were collected to 15*k* above the reference edge energy.

7.2.10 Data Reduction and Analysis

The SixPack software[11] program was used to remove bad channels, average the data, and to perform energy calibrations, in addition to data reduction and normalization. Edge normalization and background subtraction was performed using a Gaussian pre-edge function and a seven section, fourth-order polynomial spline between k = 2 Å^{-1} and k = 14 Å^{-1} for the post-edge region, followed by normalization of the edge jump.

The Artemis software program was used for EXAFS analysis by utilizing the EXAFS equation with parameters generated using FEFF6.[12,13] The EXAFS equation is defined as:

$$\chi(k) = \sum_i \frac{N_i f_i(k) e^{-2k^2\sigma_i^2}}{kr_i^2} \sin[\,2kr_i + \delta_i(k)]$$

where *f(k)* is the scattering amplitude, *δ(k)* is the phase-shift, *N* is the number of neighboring atoms, *r* is the distance to the neighboring atoms, and σ^2 is the disorder to the nearest neighbor. The data were converted to *k*-space using the relationship: $k = [\frac{2m_e(E-E_0)}{\hbar^2}]^{1/2}$. The k^3-weighted data were Fourier-transformed over a *k*-range of 2-14 Å^{-1} using a Kaisser-Bessel window for all data sets, and fit in *r*-space using an S_0 value of 0.9. The *r*-space spectra shown in figures is not phase-corrected. Data sets were fit with

separate sets of Δr_{eff} ($r - r_{eff}$) or the change in metal-ligand bond distance with respect to the input path distance and σ^2 with initial values of 0.0 Å and 0.003 $Å^2$, respectively, for the sulfur, nitrogen, and imidazole rings. Each fit was initiated with the universal E_0 (8340 eV for Ni) and an initial ΔE_0 of 0 eV, which was allowed to vary for each fit. In order to assess multiple-scattering contributions from histidine imidazole ligands, fits were performed over an *r*-space range of 1-4 Å. Histidine ligands were fit as geometrically rigid imidazole rings with varied angles of rotation, α, with α being defined as the rotation around an axis perpendicular to the plane of the ring and going through the coordinated nitrogen. In this manner, the distances of the five non-hydrogen atoms in the imidazole ring were fit in terms of a single metal-N bond distance (Δr_{eff}) for various angles (α = 0 – 10°).[14–16] Multiple-scattering parameters for imidazole ligands bound to nickel were generated using the FEFF6 software package with the initial input obtained from average bond lengths and angles gathered from crystallographic data, as previously described.[16,17] All paths with a scattering amplitude rank larger than 16 were included, where 16 is the estimated contribution of the path as calculated by Artemis.

To assess the goodness of fit from different fitting models, the fit parameters χ^2, reduced χ^2 ($r\chi^2$), and *R*-factor were minimized. Increasing the number of adjustable parameters is generally expected to improve the *R*-factor; however χ^2 may go through a minimum, the increase indicating that the model is overfitting the data. These parameters are defined as follows:

$$\chi^2 = \frac{N_{\text{idp}}}{N_{\varepsilon^2}} \sum_{N}^{i=1} \text{Re}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2 + \text{Im}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2)$$

And

$$r\chi^2 = \frac{\chi^2}{N_{\text{idp}} - N_{\text{var}}}$$

Where N_{idp} is the number of independent data points defined as $N_{\text{idp}} = \frac{(2\Delta r \Delta k)}{\pi}$, Δr is the fitting range in *r*-space, Δk is the fitting range in *k*-space, N_{ε^2} is the number of uncertainties to minimize, Re() is the real part of the EXAFS Fourier-transformed data and theory functions, Im() is the imaginary part of the EXAFS Fourier-transformed data and theory functions, and $\tilde{\chi}(R_i)$ is the Fourier-transformed data or theoretical function.

Additionally, IFEFFIT calculates the *R*-factor for each fit, which is directly proportional to χ^2 and is the root-mean-square difference between the data and calculated fit, and given by:

$$\boldsymbol{R} = \frac{\sum_{i=1}^{n}\{\mathrm{Re}[\tilde{\chi}_{data}(\mathrm{R_i}) - \tilde{\chi}_{theory}(\mathrm{R_i})]^2 + \mathrm{Im}[\tilde{\chi}_{data}(\mathrm{R_i}) - \tilde{\chi}_{theory}(\mathrm{R_i})]^2\}}{\sum_{i=0}^{n}\{\mathrm{Re}[\tilde{\chi}_{data}(\mathrm{R_i})]^2 + \mathrm{Im}[\tilde{\chi}_{data}(\mathrm{R_i})]^2\}}$$

7.3 Results

7.3.1 Protein Characterization

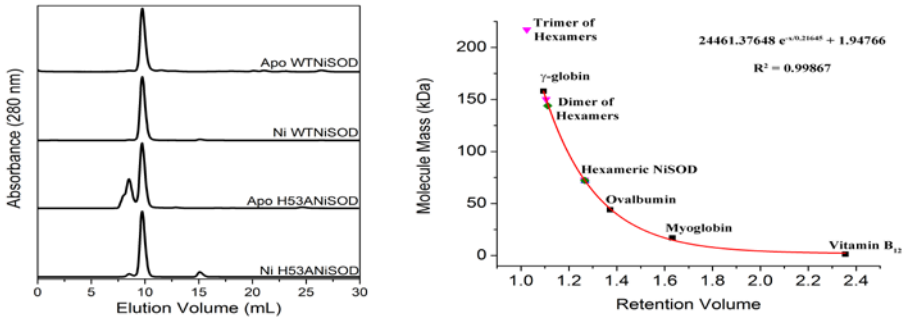

Figure 7.3: (Left) Size exclusion chromatograms for apo and holo WT- and H53A-NiSOD. (Right) Retention volume versus molecular mass for the standards and NiSOD proteins. The red line represents an exponential decay fit for the standards.

Both apo and holo WT-NiSOD displayed a molecular weight consistent with a tightly packed homohexamer as expected (**Table 7.2**).[3,5] Apo H53A-NiSOD displayed a

significant amount of higher molecular weight species which correspond to a dimer of hexamers and a trimer of hexamers, indicating that this mutation, although internal, is causing significant aggregation to occur (**Figure 7.3**). Holo H53A-NiSOD does not display this aggregation, with the primary species exhibiting a molecular weight corresponding to a tightly packed hexamer of the same molecular weight as holo WT-NiSOD. This may indicate that the nickel hook region is involved in the aggregation, although this region is disordered in the apo WT-NiSOD crystal structure and does not display aggregation. This aggregation is not reflected in the melting temperature, as the melting curve of both apo and holo H53A-NiSOD (**Figure 7.4**) consists of only one peak, with a T_m identical to WT-NiSOD (**Table 7.2**). A previous mutation in this hydrogen bonding network, D3A, is present only as a hexamer but has decreased stability as compared to WT-NiSOD.[2]

Table 7.2: Analysis of size-exclusion chromatographs and differential scanning calorimetry for apo and holo WT- and H53A-NiSOD.

Sample	Theoretical MW (kDa)	Experimental MW (kDa)	Quaternary Structure	T_m (°C)
Apo WTNiSOD	79.21	71.7	Hexamer	85.2
Ni WTNiSOD	79.56	71.8	Hexamer	86.0
Apo	78.81	72.7	Hexamer	83.6
H53ANiSOD	150.32	157.6	Dimer of Hexamers	
	217.07	236.4	Trimer of Hexamers	
Ni H53ANiSOD	79.16	72.2	Hexamer	84.1
	158.32	143.9	Dimer of Hexamers	

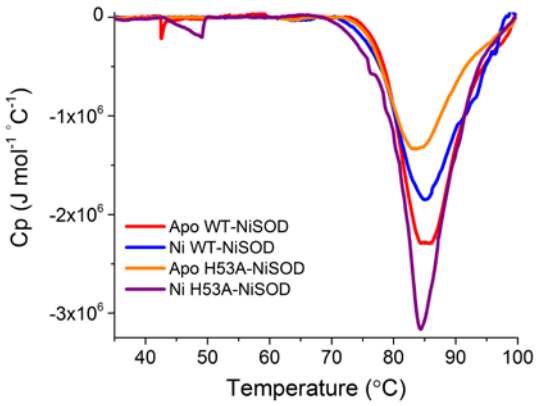

Figure 7.4: DSC thermogram of apo and holo WT- and H53A-NiSOD.

7.3.2 Kinetics

Effects of the H53A mutation on the catalytic function of NiSOD was assessed by monitoring enzyme kinetics using pulse radiolysis to generate superoxide. Pulse radiolysis generates superoxide and the rate of superoxide dismutation is measured using the absorbance of the superoxide anion at 260 nm as previously described.[1] The H53A-NiSOD mutant displays a 50% reduced catalytic rate constant (k_{calc} = 3.5 x 10^8 M^{-1} s^{-1}) as compared to WT-NiSOD (k_{calc} = 7.07 x 10^8 M^{-1} s^{-1}).[2] This is similar to what was seen for the D3A mutation which also displayed an ~50% reduction in catalytic activity.[2] The H53A-NiSOD mutation is both concentration (**Figure 7.5 Top**) and pH independent (**Figure 7.5 Middle**), properties that are unchanged as compared to WT-NiSOD. However, this mutant displays a reduced ionic strength dependence (**Figure 7.5 Bottom**), with identical catalytic rate constants compared to WT-NiSOD at high ionic strength. Previous research on CuZnSOD attributed ionic strength effects on the enzyme's function to be due to an impaired ability to guide the superoxide anion to the active site metal.[18,19]

Thus, the H53A mutation is detrimental to NiSODs ability to control the access of superoxide and other anions to the metal center.

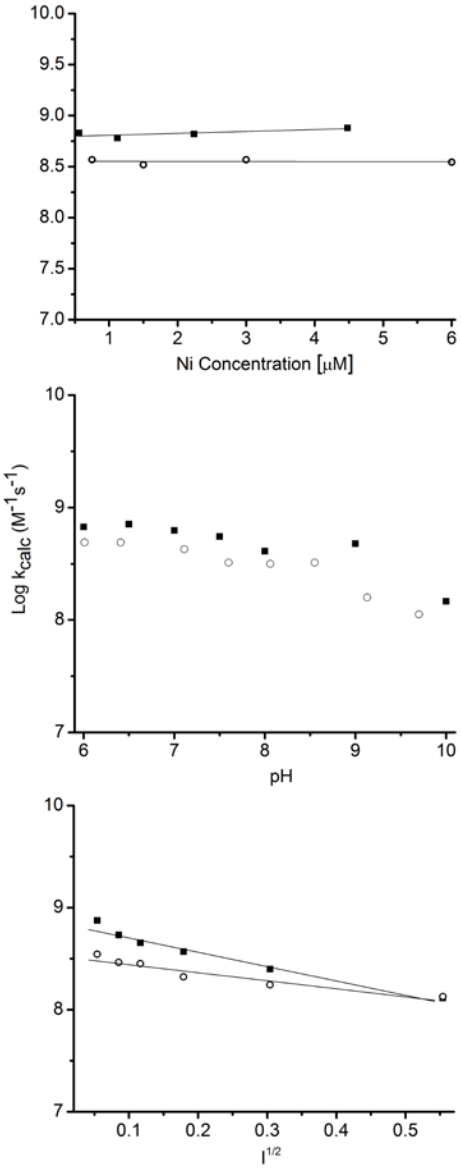

Figure 7.5: (Top) Plot of Log k_{cat} versus enzyme concentration. (Middle) Plot of Log k_{cat} versus pH. (Bottom) Plot of Log k_{cat} versus ionic strength. Closed squares represent WT-NiSOD and open circles represent H53A-NiSOD.

7.3.3 Electron Paramagnetic Resonance

EPR spectroscopy was used to probe the redox state of the enzyme and determine effects on the electronic structure of the mutant enzyme. The Ni(III) species present in

NiSOD is a low-spin square pyramidal S = ½ system with the single electron occupying the dz^2 orbital.[2,20] The X-band EPR spectrum of WT-NiSOD displays an axially distorted rhombic signal with faint N-hyperfine in the g_y and strong hyperfine in the g_z feature (A_{zz} = 24.4 G) due to the axially coordinated His1 imidazole side chain.[1,21] The EPR spectrum of H53A-NiSOD (**Figure 7.6**) reveals a line shape and g-values identical to that of WT-NiSOD (g = 2.3, 2.23, 2.01, A_{zz} = 23.5 G) indicating there has been no detectable change in the coordination of the Ni site. This is true of H53A-NiSOD oxidized with both $K_3[Fe(CN)_6]$ and $Na_2[IrCl_6]$ which coincides with previous EPR of NiSOD.[2,22]

Double integration of the Ni(III) signal in WT-NiSOD oxidized with three molar equivalents of $K_3[Fe(CN)_6]$ or $Na_2[IrCl_6]$ confirmed the previous EPR analysis wherein this signal comes from only half of the nickel centers in the sample. The H53A-NiSOD sample oxidized with three molar equivalents of $K_3[Fe(CN)_6]$ was 58% Ni(III), an increase as compared to WT-NiSOD. However, the H53A-NiSOD sample oxidized with three molar equivalents of $Na_2[IrCl_6]$ was 44% Ni(III). This discrepancy is most likely due to the EPR signal from $K_3[Fe(CN)_6]$. An initial EPR spectrum of $K_3[Fe(CN)_6]$ oxidized WT-NiSOD resulted in 72% Ni(III)[22] but this could not be reproduced in later EPR studies utilizing $K_3[Fe(CN)_6]$ as an oxidant which resulted in ~50% Ni(III) after quantification.[2] This is not unexpected, as the D3A mutation, which is also within the hydrogen bonding network containing H53, also did not allow for greater than 50% Ni(III) after oxidation. Although the D3A mutation may have been less severe in terms of disrupting cross-talk it should still have disturbed the Ni(II)/Ni(III) equilibrium. However, the EPR clearly shows that the Ni(II)/Ni(III) redox couple is unperturbed and is thus not the source of the 50% reduction in catalytic activity.

7.3.4 Electronic Structure

UV-Vis was employed to monitor changes in the electronic transitions in the H53A-NiSOD mutant (**Figure 5**). The primary electronic transitions in the UV-Vis spectrum of dithionite reduced WT-NiSOD correspond to tryptophan absorbance (~266 and 288 nm) and a S → Ni(II) charge transfer transition (311 nm).[20] The peaks corresponding to

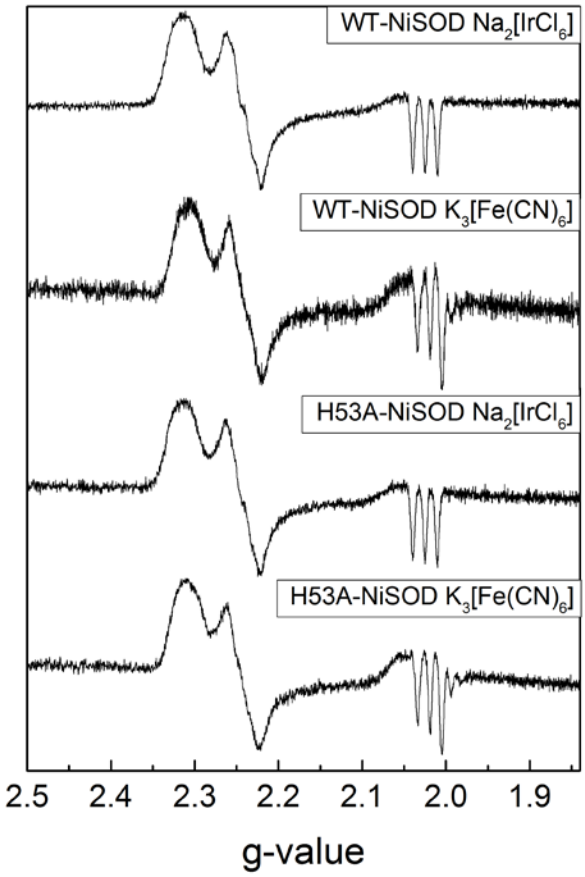

Figure 7.6: 77 K EPR spectra of WT-NiSOD and H53A-NiSOD oxidized with three molar equivalents of $Na_2[IrCl_6]$ or $K_3[Fe(CN)_6]$.

tryptophan are unchanged in the UV-Vis spectrum of dithionite reduced H53A-NiSOD indicating no change has occurred in the local environment of these residues, but there is a decrease in the extinction coefficient of the S → Ni(II) charge transfer.

Table 7.3: UV-Vis data for dithionite reduced, and as isolated WT- and H53A-NiSOD.

Sample	λ (nm)	ε (M^{-1} cm^{-1})	Sample	λ (nm)	ε (M^{-1} cm^{-1})
Reduced WT	266	22874	**Reduced H53A**	262.4	21331
	287.8	16042		280.2	16877
	311.4	10438		314	6412
As Isolated WT	276.9	17671	**As Isolated H53A**	271	18121
	320.0	4609		317.4	3758
	378.6	4242		380.4	3085

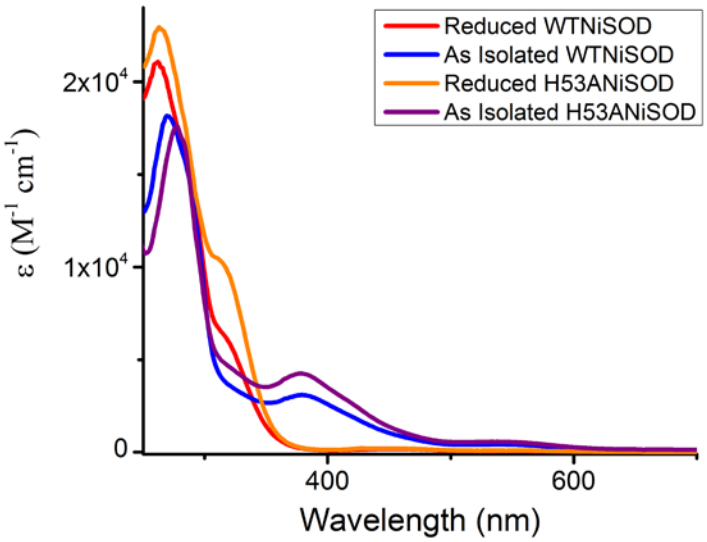

Figure 7.7: UV-Vis spectra of dithionite reduced and as isolated WT- and H53A-NiSOD.

The as isolated spectra of both WT- and H53A-NiSOD are almost identical, and consist primarily of three peaks at ~273, 318, and 379 nm. The peak at ~273 nm can be assigned tryptophan absorbance, and is slightly red shifted as compared to the reduced spectra of the enzyme, indicating that a small conformational change in the local environment of the tryptophan has occurred. The intensity of the S → Ni(II) charge transfer band is significantly diminished. The last peak at 379 nm is not present in the reduced form of the enzyme, and previous experiments have identified it as a S → Ni(III) charge transfer transition.[20] The intensity of this transition is higher in H53A-NiSOD, indicating a change in the resting oxidation state of the enzyme. As previous studies have

shown that as isolated NiSOD is 50% Ni(III), this may be indicative of a greater amount of Ni(III) present.

7.3.4 XANES Analysis

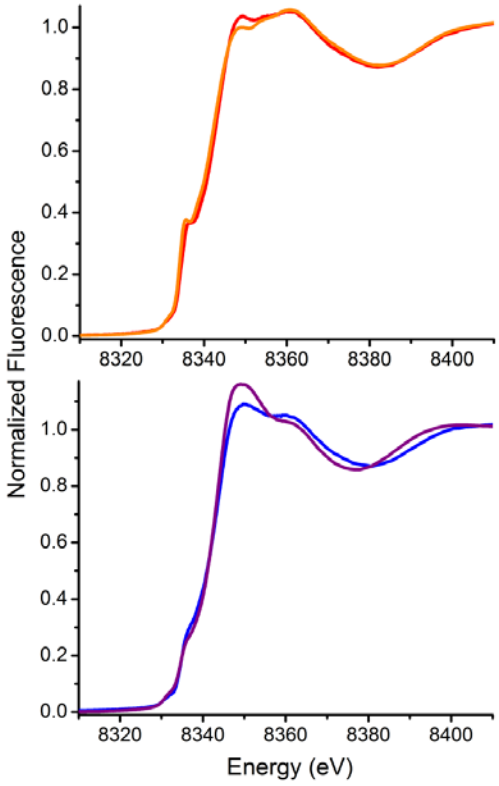

Figure 7.8: *K*-edge XAS spectra of (Top) dithionite reduced WT- (red) and H53A-NiSOD (orange) and (Bottom) as isolated WT- (blue) and H53A-NiSOD (purple) complexed to Ni(II) in buffer containing 20 mM Tris, 100 mM NaCl, and 10% glycerol at pH 8.0.

XAS studies were done on the H53A mutant to monitor any changes to the active site structure that may occur. While unlikely to occur due to the distance between the mutation and the active site (~20 Å), the reduced rate constant of this mutation may be due to structural changes. XAS was done on WT-NiSOD to allow analysis at a comparable *r*- and *k*-range to the mutant and in an attempt at analysis of the structural features seen in *r*-space between 3 and 4 Å. XAS was performed on dithionite reduced and as isolated XAS samples to monitor changes made by the mutation. The results of

XANES analysis are shown in **Table 7.4** and **Figure 7.8** and best fits obtained in EXAFS analysis are shown in **Figure 7.9** and **Figure 7.10** and summarized in **Table 7.4**.

XANES (X-ray absorption near edge structure) analysis can yield information on coordination number and geometry of the metal site. Nickel has vacancies in its 3d orbitals, allowing for a 1s → 3d transition whose intensity is dependent on the coordination number and geometry. Centrosymmetric geometries (four-coordinate planar, octahedral) produce smaller 1s → 3d transitions than non-centrosymmetric (tetrahedral, square pyramidal).[23] The 1s → $4p_z$ transition (plus shakedown) occurs when one or both axial positions are unoccupied, which can allow differentiation between geometries with similar 1s → 3d transitions (four-coordinate planar v. six-coordinate octahedral).[23] Both of these transitions are observed in the XANES spectrum of dithionite reduced WT- and H53A-NiSOD. The 1s → 3d transition is very small for both spectra (<0.5 x 10^2 eV), indicating a centrosymmetric geometry, while the 1s → $4p_z$ transition has resolved maxima in both spectra, which is characteristic of four-coordinate planar geometries.[24] For reduced WT-NiSOD this is unchanged from previous literature[1,2] and the XANES results for reduced H53A-NiSOD indicate that this mutation has not affected the geometry of the reduced sample.

The XANES of as isolated WT-NiSOD has a larger 1s → 3d peak area (5.5 ± 0.6 x 10^2 eV) than the reduced sample, which is expected because as isolated WT-NiSOD is a mixture of four-coordinate planar and square pyramidal geometries. The 1s → $4p_z$ transition is anticipated to decrease as there is now significant square pyramidal character, which has partial occupancy of one axial ligand and thus a less intense transition, and the XANES reflects this. The XANES of as isolated H53A-NiSOD has a

nearly identical 1s → 3d (5.6 ± 0.2 x 10^2 eV) as isolated WT-NiSOD which is expected for a square pyramidal geometry.[23]

7.3.4 EXAFS Analysis

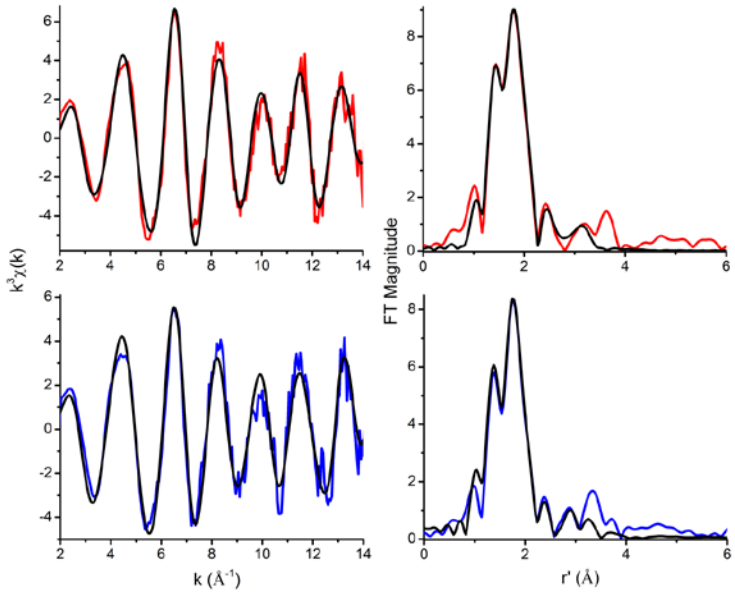

Figure 7.9: *K*-Edge EXAFS spectra of reduced (top), and as isolated (bottom) WT-NiSOD Ni(II) complexes in buffer containing 20 mM Tris, 100 mM NaCl, 10% glycerol at pH 8.0: (Left) Unfiltered k^3-weighted EXAFS spectra (colored lines) and fits (black lines). (Right) Fourier-transformed EXAFS data and fits.

The EXAFS (extended x-ray absorption fine structure) region of the XAS spectrum can provide information on the number and type of scattering atoms and their distance from the absorbing atom, which in this case is nickel. The EXAFS of WT-NiSOD was fit in order to allow comparison at equal *r*- and *k*-range, as well as to assess the change in fitting method. The best fit for reduced WT-NiSOD is similar to that previously reported, but the average Ni-N bond distance is ~2.03 Å as opposed to 1.83 Å.[2] Previous studies have found that it is difficult to obtain accurate distances for N-scattering atoms in spectra dominated by S-scattering.[23,24] This inconsistency is also seen in the high resolution crystal structures of NiSOD, with bond distances between ~1.9 – 2.2 Å being

reported for the N-terminal amine.[22,25] The best fit is additionally similar to previously reported spectra by the inclusion of a carbon atom in the second coordination sphere from the main chain carbons of His1 and Cys2. However, this fit differs in that the backscattering present between 3 – 4 Å was fit, which is present in all previously studied spectra but which has not been assigned a source.[1–3] There are no imidazoles bound in the reduced spectrum and no other possible C/N/O donor atoms within this distance. But the crystal structure of the Y9F mutation has a chloride within this distance, and this crystal structure had electron density that was unaccounted for.[2] One chloride was included in the fit that resulted in an improvement in both the %R and $r\chi^2$. This would thus indicate that chloride is present in the active site, and its position is linked to the nickel center. However, whether this is functionally relevant is unknown. The best fit for the as isolated WT-NiSOD spectrum has similar Ni-S distances to reduced WT-NiSOD (**Table 7.4**) but there is no chloride and instead there is ~0.5 imidazole ligands, consistent with previous analysis indicating an approximately equal mixture of the two geometries in the as isolated enzyme.

Table 7.4: XANES and EXAFS Analysis for Metal Complexes of WT- and H53A-NiSOD in 20 mM Tris, 100 mM NaCl, 10% glycerol, pH 8.0.

	XANES Analysis				EXAFS Analysis					
Sample	K-edge energy (eV)	$1s \rightarrow 3d$ peak area ($x10^2$ eV)	$1s \rightarrow 4p_z$ observed	Coord #/geometry	Shell	*r* (Å)	σ^2 ($x10^{-3}$ Å^2)	ΔE_0 (eV)	%R	$r\chi^2$
				WT-NiSOD						
Red Ni(II)	8334.1	<0.5	Yes	4/planar	1 N/O	1.86(1)	2(2)	-4(2)	2.8	23.9
					1 N/O	2.21(4)	7(4)			
					1 S	2.10(2)	4(2)			
					1 S	2.21(3)	6(3)			
					1 C	2.87(4)	1(4)			
					1 N/O	**1.86(1)**	**3(1)**	**-3(2)**	**2.2**	**23.0**
					1 N/O	**2.20(6)**	**6(4)**			
					1 S	**2.11(1)**	**4(2)**			
					1 S	**2.21(3)**	**5(3)**			
					2 C	**2.89(4)**	**6(5)**			
					1 Cl	**3.51(4)**	**7(5)**			
AsIsolated	8334.7	5.5(6)	Yes	5/pyramidal	1 N/O	1.85(1)	3(1)	-2(2)	3.3	26.8

Ni(II)					1 N/O	2.10(2)	8(1)			
					1 S	2.10(1)	6(1)			
					1 S	2.24(1)	3(1)			
					2 C	2.92(3)	5(4)			
					1 N/O	**1.83(2)**	**2(1)**	**-6(2)**	**3.0**	**29.3**
					1 N/O	**2.26(2)**	**9(1)**			
					1 S	**2.11(1)**	**5(1)**			
					1 S	**2.24(2)**	**7(1)**			
					2 C	**2.85(7)**	**10(11)**			
					0.5 Imd	**1.89(9)**	**5(10)**			
					1 N/O	1.85(2)	2(1)			
					1 N/O	2.13(3)	7(2)			
					1 S	2.13(3)	4(2)			
					1 S	2.24(3)	1(4)			
					2 C	2.88(4)	5(6)			
					0.5 Imd	1.98(3)	2(2)			
					1 Cl	3.45(16)	24(30)			
				H53A-NiSOD						
Red Ni(II)	8334.1	<0.5	Yes	4/planar	1 N/O	1.86(1)	2(1)	-2(2)	2.2	133
					1 N/O	2.26(2)	9(2)			
					1 S	2.11(1)	5(1)			
					1 S	2.24(2)	7(1)			
					2 C	2.90(4)	8(5)			
					1 N/O	**1.86(1)**	**2(1)**	**-2(1)**	**1.7**	**123**
					1 N/O	**2.26(2)**	**9(1)**			
					1 S	**2.11(1)**	**5(1)**			
					1 S	**2.24(1)**	**7(1)**			
					2 C	**2.90(4)**	**8(5)**			
					1 Cl	**3.50(4)**	**10(6)**			
AsIsolated Ni(II)	8334.7	5.6(2)	Yes	5/pyramidal	1 N/O	1.85(1)	1(1)	-5(2)	5.5	20.5
					1 N/O	2.10(1)	9(1)			
					1 S	2.10(1)	6(1)			
					1 S	2.26(2)	3(1)			
					4 C	2.89(4)	12(5)			
					1 N/O	**1.84(2)**	**1(2)**	**-4(2)**	**4.8**	**21.4**
					1 N/O	**2.12(3)**	**5(3)**			
					1 S	**2.11(2)**	**3(2)**			
					1 S	**2.26(2)**	**0(2)**			
					4 C	**2.87(3)**	**8(3)**			
					0.5 Imd	**2.00(2)**	**2(1)**			
					1 N/O	1.85(2)	0(2)	-4(2)	4.5	25.1
					1 N/O	2.12(4)	5(3)			
					1 S	2.11(3)	3(2)			
					1 S	2.26(2)	0(2)			
					4 C	2.87(3)	8(3)			
					1 Cl	3.43(15)	23(27)			
					0.5 Imd	2.00(2)	3(1)			

The best EXAFS fit of reduced H53A-NiSOD is identical in all respects to the best WT fit. This confirms that this mutation has not affected the nickel site structure, which is expected as His53 is ~20 Å away from the nickel center. The best fit of as isolated H53A-NiSOD EXAFS spectrum is again nearly identical to that of WT-NiSOD, except

that one of the nitrogens is much shorter (2.26 Å to 2.12 Å) and the imidazole distance is longer (1.89 Å to 2.00 Å). However, as previously stated, it can be difficult to obtain accurate nitrogen bond distances in spectra dominated by sulfur scattering. What is clear is that this mutation does not affect the nickel site structure in either the reduced or as isolated state.

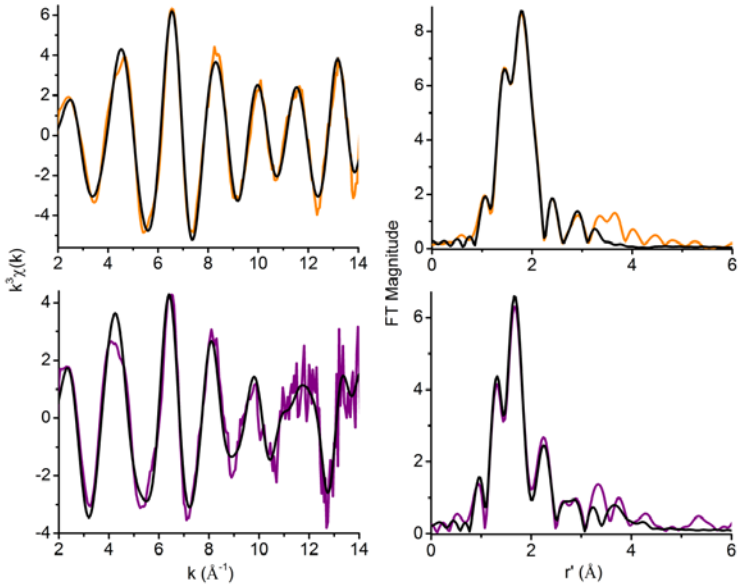

Figure 7.10: Ni *K*-Edge XAS spectra of reduced (top), and as isolated (bottom) H53A-NiSOD nickel complexes in buffer containing 20 mM Tris, 100 mM NaCl, 10% glycerol at pH 8.0: (Left) Unfiltered k^3-weighted EXAFS spectra (colored lines) and fits (black lines). (Right) Fourier-transformed EXAFS data and fits.

7.4 Conclusion

NiSOD Active Site Cross-Talk. One of the most unusual features of NiSOD is that it is isolated as 50% Ni(II) and 50% Ni(III), indicating that three monomers in the hexamer are either resistant or inaccessible to oxidants.[1,2] This again assumes that the Ni(III) signal seen is due to a half-oxidized/reduced hexamer, and not that half the hexamers in the sample are oxidized and half reduced. NiSOD is a homohexamer whose individual

active sites appear to be identical and equally solvent accessible by crystallography. If all sites are identical this would indicate that if half of the active sites are available for oxidation, then all of them must be available for oxidation. This is not the case, thus leading to the conclusion that half of the protein is resistant to oxidation, rather than inaccessible. This resistance would suggest that the oxidation state of one nickel center is transmitted to an adjacent nickel center, ensuring that the protein does not exceed 50% oxidation as monitored with current experimental techniques. Because the active sites appear to be equal it is expected that the nickel centers exert equal influence on each other, i.e. either member of the pair is available for oxidation and only when oxidation occurs is the adjacent nickel center prevented from oxidation. One possible mode of communication was proposed to occur via a symmetrical hydrogen bonding network, of which there are only two in NiSOD. One hydrogen bonding network, involving Glu17 and Arg47,[3] has been previously studied and does not allow for oxidation higher than 50%. The other hydrogen bonding network is the subject of this work and involves His53.

However, it is apparent from the EPR results in which there is no increase in Ni(III) character as compared to WT-NiSOD that the disruption of the hydrogen bonding network involving His53 is not responsible for controlling the amount of Ni(III) present. As there are no other symmetrical hydrogen bonding networks connecting the nickel centers within this enzyme the only other explanation is that all the nickel sites are not equal. This could be explained by 1) half of the nickel centers are actually solvent inaccessible or 2) there is an unsymmetrical hydrogen bonding network that controls the redox state of each nickel center. The first conclusion is not supported by crystallographic

data. However, it cannot be completely ruled out, as NiSOD enzyme used for crystallography is not catalytically primed. During pulse radiolysis on enzyme that has not been previously subjected to superoxide, the initial spectrum displays a two-exponential decay rate, which consists of an initial ultra-fast species and a secondary decay rate which corresponds to superoxide dismutation. Examining primed or other possible 'active' forms and other mechanisms for controlling the amount of Ni(III) could be the focus of future investigations.

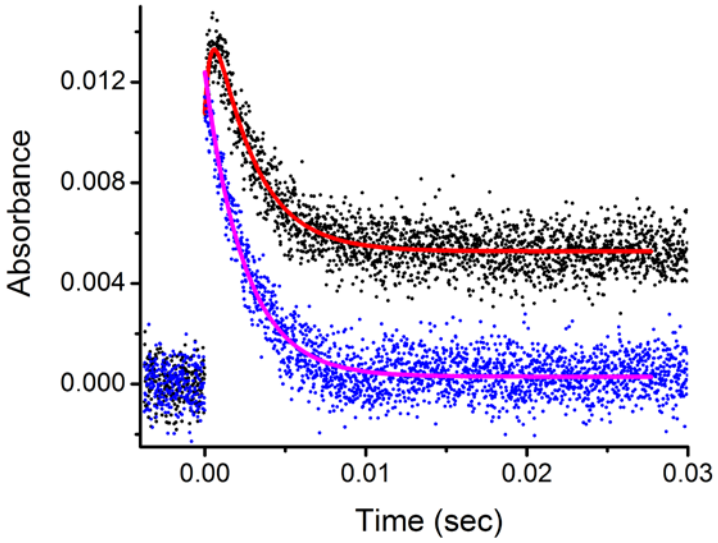

Figure 7.11: Kinetic traces monitoring the absorbance at 260 nm. First pulse (black) with double exponential decay fit (red) overlaid with second pulse (blue) with first order exponential fit (pink).

This initial two-exponential decay rate is not visible again on any subsequent experiments which only display a first-order exponential, but is reproducible on fresh enzyme. It is possible that NiSOD undergoes a permanent internal reordering upon interaction with superoxide. The second explanation (there is an unsymmetrical hydrogen bonding network) is more plausible only by virtue of having no evidence to disprove it,

although how a symmetrical protein would generate a non-symmetrical hydrogen bonding network is a point of contention.

However, this work makes it clear that the effects of the D3A mutation were not caused solely by disruption of the second coordination sphere, but were caused by disruption of this hydrogen bonding network. The H53 residue is ~20 Å away from the active site but still causes a ~50% reduction in catalytic activity. This mutation causes aggregation in the apo protein and has impaired the guidance of anions to the active site. Thus the whole protein is involved in modulating the catalytic activity of the active site and not simply the first and second coordination sphere.

Electrostatic Guidance of Superoxide. The H53A mutation has not been shown to disrupt cross-talk between nickel centers. Regardless, this mutation decreases the catalytic rate by 50%, indicating that it is important for enzyme function despite its distance from the metal center. This mutation remains independent of both concentration and pH, so it is not involved in the transfer of either proton and the mechanism remains independent of substrate concentration. However, this mutation was shown to have affected ionic strength dependence. Previous studies on CuZnSOD have determined that the ionic strength of the buffer interferes with the electrostatic guidance of the superoxide anion to the redox active metal center.[7,18,19] Thus, this mutant enzyme could be deficient in electrostatic guidance, which may account for the decreased catalytic activity and explain why the mutant overlaps with the WT enzyme at high salt concentration. The results of the XAS studies indicate that instead of competition or interference by buffer anions, chloride ions may be a functional feature of the active site pocket. While chloride ions have been shown to be present in the NiSOD active site by both the crystal structures

and now by XAS there is no difference between the XAS structures of WT-NiSOD and H53A-NiSOD, indicating that interference with the electrostatic guidance is occurring outside the active site.

7.5 References

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APPENDIX A

CIRCULAR DICHROISM MELTS and β-GALACTOSIDASE ASSAYS FOR RCNR

A.1.1 Circular Dichroism

Temperature scans (40 – 100 °C at 222 nm, 1 mm path length) were carried out on a Jasco J-1500 CD spectrometer. Wavelength scans (20 nm/min, 2 nm step size) and temperature scans (1 °C/min) were performed on 20 μM apo-WT-RcnR protein and the variants, and 20 μM metal-substituted WT-RcnR protein and the variants in buffer (10 mM Hepes, 150 mM NaCl, 5% glycerol at pH 7.0) that was allowed to equilibrate with 1 equiv of metal for 4 h. Each spectrum was the accumulation of four scans, and the background buffer scans were subtracted from each spectrum. Reverse scans were performed and melting is reversible in all cases. Baseline correction and normalization was performed in Origin, and midpoints were taken as melting temperatures, $T_{m,}$ except in cases where maxima were not observed, where the limit of the curves obtained placed a lower limit on the values of T_m.

A.1.2 β-galactosidase assays

All the data in this section were handled as outlined in Chapter 2, Section 2.2.6.

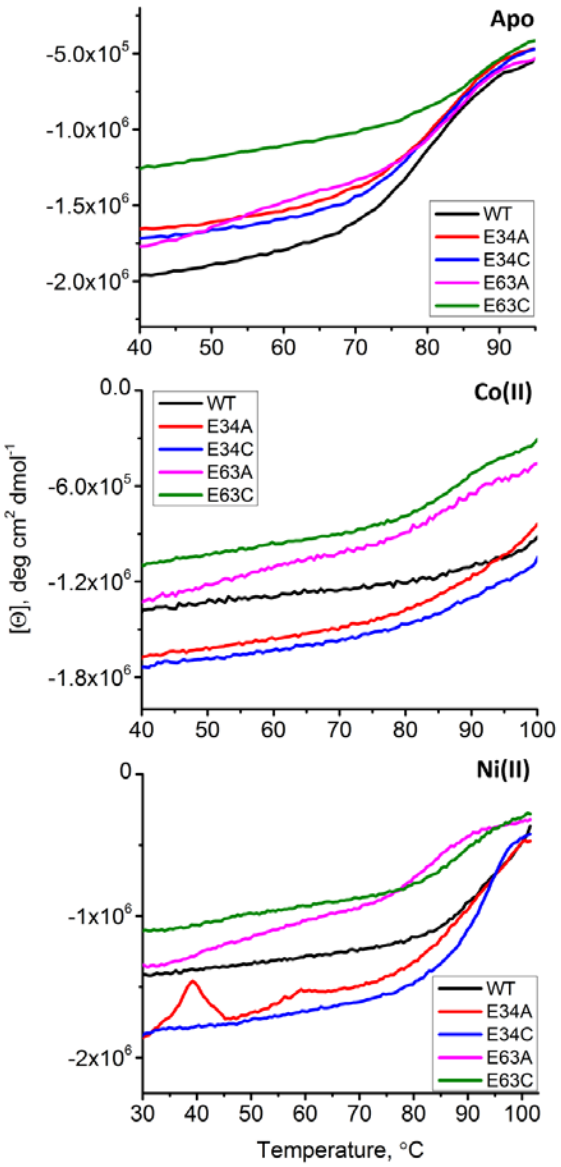

Figure A.1: Circular dichroism temperature melts of WT RcnR and variants in 20 mM HEPES, 150 mM NaCl, 5% glycerol, pH 7.0. Top Spectrum: Apo WT-RcnR and variants. Middle Spectrum: WT-RcnR and variants with 2 molar equivalents of $CoCl_2$. Bottom Spectrum: WT-RcnR and variants with 2 molar equivalents of $NiCl_2$.

A.2 E34 Temperature Melt Results

Thermal denaturation measurements were performed on the Glu34 variants of RcnR with and without metal ions in order to monitor changes in thermal stability as judged by

Table A.1: Melting Temperature of WT and Mutant RcnR Proteins in 20 mM HEPES, 100 mM NaCl, 5% Glycerol, pH 7.0.

Sample	Apo T_m (°C)	+Co T_m (°C)	+Ni T_m (°C)
WT	80.0	>100	>100
E34A	81.7	>100	93.1
E34C	81.4	>100	92.8

T_m values (**Table A.1**). Apo WT-RcnR melts at 80 ^oC, and upon addition of both Ni(II) and Co(II) the melting temperature increases by >20 ^oC, consistent with previous reports (**Table A.1**).[1] Apo E34A- and E34C-RcnR have melting temperatures of 82 ^oC and 81 ^oC, respectively, very similar to WT-RcnR. Upon the addition of Co(II) to the Glu34 variants, the melting temperatures both increase by >20 ^oC, similar to WR-RcnR. However, upon the addition of Ni(II) a smaller increase in T_m of ~12 ^oC is observed. Nonetheless, large increases in T_m are observed upon cognate metal binding to Glu34 variants. These differences in thermal stability correlate well with changes in transcriptional response (**Figure 2.5**), with small increases in thermal stability being associated with decreased transcriptional response (*vide infra*). However, whether thermal stability is truly the cause of the functional differences cannot be definitively stated.

A.3 E63 Temperature Melts

Thermal denaturation measurements were performed on the Glu63 variants of RcnR with and without metal ions in order to monitor changes in thermal stability as judged by T_m values (Table 3.2). Apo WT-RcnR melts at 80 ^oC, and upon addition of both Ni(II) and Co(II) the melting temperature increases by >20 ^oC, consistent with

previous reports (Table 3.2).[1] Apo E63A-and E63C-RcnR variants melt at 83 ^{o}C and 87°C, respectively, and thus exhibit slight *increases* in stability relative to WT-RcnR. Further, increases of only ~5 °C and ~1 °C are observed upon binding Co(II), and increases of < ~2 °C are observed upon binding Ni(II). Thus, the Glu63 variants do not exhibit the increases in T_m that are characteristic of WT-RcnR or the Glu34 variants. These differences in thermal stability correlate well with changes in transcriptional response (**Table A.2, Figure 3.4**), with small increases in thermal stability upon metal binding being associated with decreased transcriptional response (*vide infra*).

Table A.2: Melting Temperature of WT and Mutant RcnR Proteins in 20 mM HEPES, 100 mM NaCl, 5% Glycerol, pH 7.0.

Sample	Apo T_m (°C)	+Co T_m (°C)	+Ni T_m (°C)
WT	80.0	>100	>100
E63A	82.8	87.3	82.3
E63C	87.0	88.3	89.2

A.4 Tables of Raw β-galactosidase Results

Table A.3: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E34A-RcnR.

	Miller Units							
	Trial 1A	Trial1B	Trial 2A	Trial 2B	Trial 3A	Trial 3B	Trial 4A	Trial 4B
Apo WT-RcnR	3.64	3.58	2.59	2.72	3.04	3.01	2.85	2.80
Co WT-RcnR	49.01	47.31	56.55	55.64	63.54	63.08	58.80	57.77
Ni WT-RcnR	40.45	43.23	38.61	40.13	66.96	61.70	61.89	60.21
Zn WT-RcnR	2.84	2.84	2.14	2.55	3.35	3.55	3.31	3.52
Apo E34A-RcnR	2.54	2.53	3.29	3.12	3.76	3.67	4.08	4.18
Co E34A-RcnR	52.72	51.15	51.64	50.08	58.98	62.33	58.10	57.37
Ni E34A-RcnR	46.89	47.49	45.21	46.19	63.11	61.43	59.67	63.90
Zn E34A-RcnR	2.85	2.82	3.42	2.94	3.43	3.16	3.38	3.68

Table A.4: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E34C-RcnR.

	Miller Units							
	Trial 1A	Trial1B	Trial 2A	Trial 2B	Trial 3A	Trial 3B	Trial 4A	Trial 4B
Apo WT-RcnR	2.21	2.32	1.98	2.01	3.11	3.16	3.65	3.63
Co WT-RcnR	57.75	54.13	50.85	48.44	59.68	59.59	66.55	66.12
Ni WT-RcnR	52.74	53.26	48.92	50.93	55.43	57.98	64.67	69.00
Zn WT-RcnR	2.34	2.29	2.08	1.96	3.17	3.18	3.09	3.31
Apo E34C-RcnR	2.10	1.79	2.64	3.41	2.96	2.92	4.04	4.13
Co E34C-RcnR	54.34	54.28	53.13	50.25	47.02	46.88	50.18	51.37
Ni E34C-RcnR	48.16	45.67	46.62	48.83	43.77	44.80	53.45	52.35
Zn E34C-RcnR	1.99	2.13	2.69	2.61	2.73	2.70	2.86	2.78

Table A.5: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E63A-RcnR.

	Miller Units							
	Trial 1A	Trial1B	Trial 2A	Trial 2B	Trial 3A	Trial 3B	Trial 4A	Trial 4B
Apo WT-RcnR	2.39	2.47	3.13	3.20	3.40	3.41	2.89	3.04
Co WT-RcnR	46.99	46.60	53.33	52.34	76.73	76.38	62.97	62.14
Ni WT-RcnR	43.31	43.15	51.47	50.57	85.53	78.76	63.88	63.44
Zn WT-RcnR	2.32	2.19	2.72	2.96	2.98	2.95	3.15	3.16
Apo E63A-RcnR	2.65	2.66	3.82	3.88	4.03	4.25	5.11	4.13
Co E63A-RcnR	42.26	42.58	56.22	55.47	25.84	25.15	60.25	59.31
Ni E63A-RcnR	22.95	23.13	27.98	27.68	56.08	57.21	30.18	29.97
Zn E63A-RcnR	2.65	2.59	3.72	3.59	2.72	3.28	3.58	3.49

Table A.6: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E63C-RcnR.

	Miller Units							
	Trial 1A	Trial1B	Trial 2A	Trial 2B	Trial 3A	Trial 3B	Trial 4A	Trial 4B
Apo WT-RcnR	2.67	2.65	2.83	2.86	2.81	2.71	2.73	2.73
Co WT-RcnR	58.71	59.06	59.43	58.38	52.07	50.20	50.38	49.01
Ni WT-RcnR	58.14	57.34	59.21	56.91	51.66	50.54	52.87	51.99
Zn WT-RcnR	2.38	2.33	2.47	2.47	2.54	2.49	2.46	2.34
Apo E63C-RcnR	4.13	4.17	3.94	3.72	3.01	3.14	3.05	2.97
Co E63C-RcnR	47.06	45.86	45.73	46.11	31.73	31.59	32.12	32.11
Ni E363C-RcnR	34.14	32.29	35.49	33.77	23.11	22.60	21.54	22.66
Zn E63C-RcnR	3.70	3.61	3.50	3.44	3.12	3.04	2.86	2.95

Table A.7: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E34A-RcnR titrated with different amounts of $Co(Ac)_2$.

μM $Co(Ac)_2$	0	10	30	50	70	90	110	130	180
WT-RcnR Trial One	5.06	14.94	47.87	60.84	67.93	77.05	81.01	82.69	86.69
WT-RcnR Trial Two	3.95	15.99	46.58	61.86	70.29	74.01	78.47	81.44	87.40
WT-RcnR Trial Three	2.00	9.18	35.86	44.74	44.89	59.11	61.89	65.19	71.35
WT-RcnR Trial Four	2.75	12.14	40.98	48.29	51.38	67.07	72.46	74.23	83.86
E34A-RcnR Trial One	6.47	14.07	48.69	45.00	49.77	52.73	55.88	53.42	55.05
E34A-RcnR Trial Two	7.44	17.28	53.85	70.81	78.87	77.01	82.57	85.20	84.26
E34A-RcnR Trial Three	2.62	7.42	35.92	45.40	49.79	62.90	64.75	72.74	66.17
E34A-RcnR Trial Four	2.21	6.45	33.59	42.64	45.44	56.27	57.52	60.89	67.31

Table A.8: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E34C-RcnR titrated with different amounts of $Co(Ac)_2$.

μM $Co(Ac)_2$	0	10	30	50	70	90	110	130	180
WT-RcnR Trial One	4.73	17.96	48.97	65.80	78.86	85.10	91.05	94.74	96.83
WT-RcnR Trial Two	4.44	15.19	50.57	70.69	85.32	94.81	94.46	94.37	104.13
WT-RcnR Trial Three	2.97	5.85	36.54	46.92	47.05	57.21	60.80	60.05	62.78
WT-RcnR Trial Four	2.84	6.00	38.99	45.70	46.42	51.42	53.90	58.37	60.60
E34C-RcnR Trial One	5.51	12.87	41.71	58.25	62.38	69.74	73.25	76.06	86.84
E34C-RcnR Trial Two	7.06	16.10	42.82	58.78	64.81	75.25	75.74	75.46	81.94
E34C-RcnR Trial Three	3.87	9.29	32.62	46.05	49.20	59.86	61.84	65.83	70.41
E34C-RcnR Trial Four	3.76	9.72	32.91	46.38	51.32	57.66	60.58	57.09	58.90

Table A.9: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E34A-RcnR titrated with different amounts of $Ni(Ac)_2$.

μM $Ni(OAc)_2$	0	100	200	300	400	500	600	700	900
WT-RcnR Trial One	4.48	4.70	5.49	11.99	25.70	45.72	58.82	72.11	78.99
WT-RcnR Trial Two	4.71	4.83	5.16	12.60	25.46	45.57	63.03	60.69	85.08
WT-RcnR Trial Three	4.93	5.14	6.45	19.80	42.04	69.96	81.85	95.46	108.63
WT-RcnR Trial Four	4.60	5.05	5.78	17.60	34.86	61.19	63.06	78.04	119.48
E34A-RcnR Trial One	3.81	4.20	4.78	10.03	21.63	38.71	54.16	61.68	73.32
E34A-RcnR Trial Two	3.72	4.03	4.87	10.89	21.60	38.98	51.36	78.11	86.23
E34A-RcnR Trial Three	9.15	10.01	13.35	20.23	45.20	80.23	91.34	104.6	114.31
E34A-RcnR Trial Four	6.63	7.24	8.59	14.91	28.43	47.68	56.23	78.07	104.60

Table A.10: β-galactosidase results of Trials 1-4 and the internal replicates for WT- and E34C-RcnR titrated with different amounts of $Ni(Ac)_2$.

μM $Ni(OAc)_2$	0	100	200	300	400	500	600	700	900
WT-RcnR Trial One	4.61	4.86	5.32	13.51	21.16	41.66	61.39	80.06	88.36
WT-RcnR Trial Two	4.13	4.26	4.52	11.30	16.99	37.30	50.17	71.49	84.45
WT-RcnR Trial Three	6.72	7.02	7.96	10.70	39.24	64.75	98.41	155.22	145.97
WT-RcnR Trial Four	5.50	4.93	5.13	6.83	26.87	55.84	71.37	99.06	117.77
E34C-RcnR Trial One	7.28	7.20	7.42	10.03	18.89	33.52	60.26	78.75	99.89
E34C-RcnR Trial Two	6.72	7.16	6.62	8.60	16.84	30.39	51.69	70.01	91.18
E34C-RcnR Trial Three	9.02	9.28	10.10	12.87	30.72	55.82	66.69	89.88	110.99
E34C-RcnR Trial Four	7.45	7.98	8.47	10.98	24.01	41.73	56.58	72.07	95.81

APPENDIX B

NONOATE BOUND TO NISOD

B.1 Expression, Purification and Processing of WT-NiSOD

Single colonies were grown overnight at 37 ºC with shaking in 10 mL Luria-Bertani broth, supplemented with chloramphenicol (cam) and kanamycin (kan) for selection. These cultures were added to 1 L pre-warmed fresh media and grown to an OD_{600} nm of 0.6 and then induced with 0.8 mM isopropyl β-D-1-thiogalactopyranoside (IPTG) for 3-5 hours. Cells were harvested by centrifugation, resuspended in 40 mL Ni-NTA binding buffer (10 mM imidazole, 50 mM tris, 300 mM sodium chloride pH 8.0), and then frozen at -80 ºC to lyse the cells. The lysed cell harvests were thawed and treated with 100 μL of DNAse I solution (10 mg/ml DNAse I, 10 mM magnesium chloride, 20 mM Tris pH 7.5, 40% glycerol) at 37 ºC until the viscosity of the solution was significantly reduced. The cell lysate was centrifuged for 5 min at 8,000 rpm and the supernatant was used for protein purification.

All chromatographic purifications employed an AKTA-FPLC (Amersham Biosciences). The cell lysate supernatant was loaded onto a column (Pharmacia HR10) containing Ni-NTA HisBind Superflow™ resin (Novagen™) at 3 ml/min with Ni-NTA binding buffer. Once the absorbance at 280 nm returned to the baseline, the buffer was changed to 33% elute buffer (250 mM imidazole, 50 mM Tris, 300 mM sodium chloride pH 8.0) in one step, and the column was washed with 7 column volumes of 33% elute buffer. The fusion protein was then eluted from the column using 100% elute buffer.

Electrospray ionization mass spectroscopy (ESI-MS) was used to confirm the molecular weight (MW) of the expected fusion protein.

The purified fusion protein was N-terminally processed to yield NiSOD with the WT N-terminus by using factor Xa. The fusion protein was buffer exchanged three times with 20 mM Tris buffer pH 8.5 and then seven times with factor Xa cleavage buffer (5 mM calcium chloride, 50 mM Tris, 100 mM sodium chloride, pH 8.0). The concentration of fusion protein in factor Xa cleavage buffer was determined using a bicinchoninic acid (BCA) assay. The assay was performed using the Enhanced Test Tube Protocol outlined in Pierce's BCA™ Protein Assay Kit instruction manual. Factor Xa was then added (1 unit/50 μg fusion protein) and the mixture was incubated at 4 ºC. The extent of cleavage was monitored using 16% SDS-PAGE.

B.2 EPR Spectroscopy

A 100 μL sample containing 500 μM Apo WT-NiSOD in 50 mM Tris, 200 mM NaCl, pH 8.0 was prepared. Freshly prepared NONOate (100 mM) in 10 mM NaOH and DTT (500 mM) in 50 mM Tris, 200 mM NaCl, pH 8.0 were added to the samples such that the final volumes were 100 μL and the final concentrations were 500 μM (1 molar equivalent compared to WT-NiSOD). The samples were transferred to EPR tubes and flash frozen in liquid nitrogen. EPR samples were run using a finger dewar on a Bruker Elexsys E-500 EPR equipped with a DM4116 cavity at 9.639 GHz frequency, 20.31 200 mW power, 10G modulation amplitude, 100 GHz modulation frequency, 5.12 ms time constant, 77K.

B.3 Introduction

It is now know that nitric oxide is a highly prevalent signaling molecule and can be found as a signaling molecule in every cell type within mammals.[2] In addition to acting as a signaling molecule in the gaseous form, nitric oxide can also react with cysteines to form S-nitrosothiols[3] that is a prevalent form of post-translational modification that is not only a signal in and of itself, but is reversible[4,5]. Thus S-nitrosothiol generation can allow the transport of nitric oxide to another area of the cell/organism before nitric oxide release occurs. It is currently thought that much of the modification (oxidation, S-nitrosylation, etc) that has been observed in cysteines serves a regulatory purpose.

The purpose of this experiment was to see if Apo WT-NiSOD could trap and stabilize the nitric oxide radical. Because the cysteines are not oxidized during superoxide disproportionation it is possible that they are resistant to oxidation even in the absence of nickel. Instead of reacting with nitric oxide, the cysteines, in conjunction with a nearby positively charged residue, would be able to form ionic bonds with nitric oxide due to its dipole moment. An example of one such bond is shown in **Figure B.1,** where nitric oxide is between Cys2 and a nearby arginine residue with the negatively charged nitrogen interacting with the positive arginine and the negatively charged cysteine interacting with the partial positive charge of the oxygen.

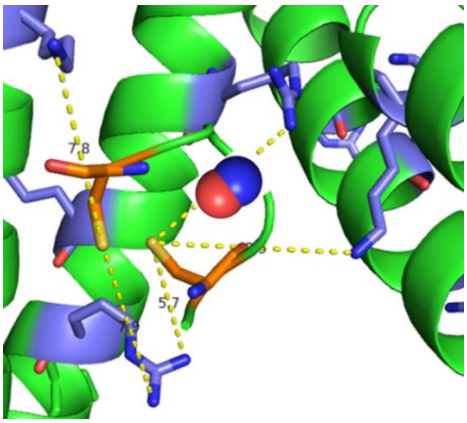

Figure B.1: Close up view of the active site of WT-NiSOD (PDB ID: 1T6U) without nickel. Dashed lines represent bonds between cysteines (orange) and nearby positively charged residues (blue). Nitric oxide (red and blue spheres) shown to represent proposed mode of binding.

B.4 EPR Results

Figure B.2 shows the results of the EPR studies. Nitric oxide by itself has a broad and indistinct EPR signal in aqueous solutions[6] as seen below and thus is a major contribution as to why it is not detected via EPR in biological samples without a method of trapping such as binding to heme. NONOate reaction with DTT was performed as a control because it is thought that apo WT-NiSOD forms a disulfide bond between Cys2 and Cys6, precluding nickel binding to the active site. However, addition of DTT quenches the reaction, most likely via formation of S-nitrosyl species that are EPR silent but visible by UV-Vis spectroscopy.[7] Addition of NONOate to NiSOD causes the formation of a defined EPR signal which is dissimilar to sulfur radicals, which typically have a g-value of 2.0 (g-value of NiSOD-NO species is 2.4).[8] Addition of DTT causes the signal to disappear, indicating that the signal seen in the NiSOD-NO spectrum is not covalent and thus does not protect nitric oxide from being scavenged by DTT to form an S-nitrosyl species. Based on these preliminary experiments, NiSOD can indeed stabilize

nitric oxide and can act as a sensor for nitric oxide without formation of another species or binding to a metal sensor, which are the current standard for nitric oxide sensing.

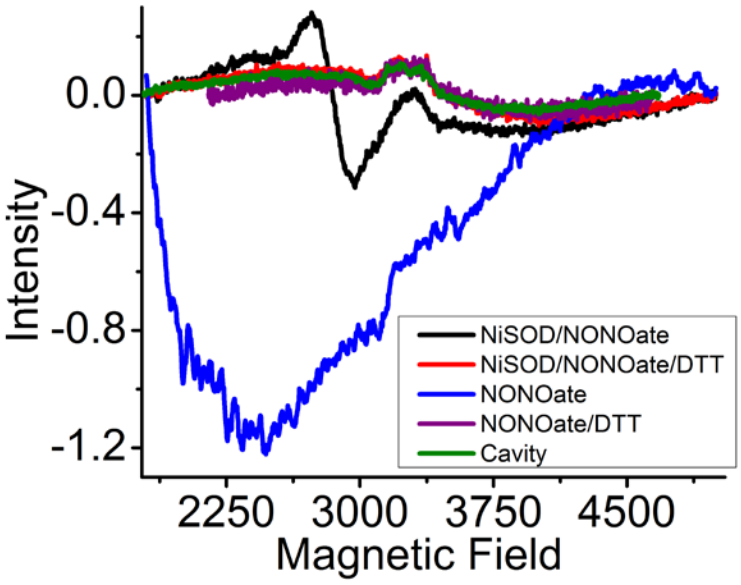

Figure B.2: Experimental X-Band EPR spectra of NONOate - NiSOD complexes in 50 mM Tris, pH 8.0: 500 μM NONOate (blue), 500 μM NONOate with 500 μM DTT (purple), 500 μM Apo WT-NiSOD with 500 μM NONOate (black), and 500 μM Apo WT-NiSOD with 500 μM NONOate and DTT (red), 9.639 GHz frequency, 200 mW power, 10G modulation amplitude, 100 GHz modulation frequency, 512 ms time constant, 77 K.

APPENDIX C

PHD2 XAS

C.1 XAS

XAS data collection for all samples was performed on beam line X3B at the National Synchrotron Light Source (NSLS), Brookhaven National Laboratories (Upton, NY). The samples were cooled to ~50 K using a He displex crysostat, and data was collected under ring conditions of 2.8 GeV and 120-300 mA using a sagittally focusing Si(111) double-crystal monochromater. X-ray fluorescence was collected using a 30-element Ge detector (Canberra). Scattering was minimized by placing a Z-1 filter between the sample chamber and the detector.

Internal energy calibration was performed by collecting spectra simultaneously in transmission mode on the corresponding metal foil to determine the first inflection point on the edge, which was set to 8331.6 eV for Ni, or 9660.7 eV for Zn. X-ray absorption near-edge structure (XANES) data were collected from -200 to +200 eV relative to the metal K-edge. Extended X-ray absorption fine structure (EXAFS) data were collected to 15*k* above the reference edge energy.

C.2 Data Reduction and Analysis

The SixPack software[9] program was used to remove bad channels, average the data, and to perform energy calibrations, in addition to data reduction and normalization. Edge normalization and background subtraction was performed using a Gaussian pre-edge function and a seven point quadratic polynomial spline between $k = 2$ Å^{-1} and $k = 14$ Å^{-1} for the post-edge region, followed by normalization of the edge jump.

The Artemis software program was used for EXAFS analysis with parameters generated using FEFF6 and scattering paths were fit the IFFEFIT engine.[10,11] The data were converted to *k*-space using the relationship: $k = [\frac{2m_e(E-E_0)}{\hbar^2}]^{1/2}$. The k^3-weighted data were Fourier-transformed over a *k*-range of 2-12.5 $Å^{-1}$ using a Kaisser-Bessel window for all data sets, and fit in *r*-space using an S_0 value of 0.9. The r-space spectra shown is not phase-corrected. Data sets were fit with separate sets of Δr_{eff} and σ^2 for the sulfur, nitrogen, and imidazole rings with initial values of 0.0 Å and 0.003 $Å^2$, respectively. Each fit was initiated with the universal E_0 (8340 eV for Ni, and 9670 eV for Zn) and an initial ΔE_0 of 0 eV, which was allowed to vary for each fit. In order to assess multiple-scattering contributions from histidine imidazole ligands, fits were performed over an *r*-space range of 1-4 Å. Histidine ligands were fit as geometrically rigid imidazole rings with varied angles of rotation, α, with α being defined as the rotation around an axis perpendicular to the plane of the ring and going through the coordinated nitrogen. In this manner, the distances of the five non-hydrogen atoms in the imidazole ring were fit in terms of a single metal-N bond distance (Δr_{eff}) for various angles (α = 0 – 10°).[12–14] Multiple-scattering parameters for imidazole ligands bound to nickel, cobalt and zinc were generated using the FEFF6 software package with the initial input obtained from average bond lengths and angles gathered from crystallographic data, as previously described.[14,15] All paths with relative amplitudes larger than 16% of the pathway with maximum intensity were included.

To assess the goodness of fit from different fitting models, the fit parameters χ^2, reduced χ^2 ($r\ \chi^2$), and *r*-factor were minimized. Increasing the number of adjustable parameters is generally expected to improve the *r*-factor; however χ^2 may go through a

minimum, the increase indicating that the model is overfitting the data. These parameters are defined as follows:

$$\chi^2 = \frac{N_{\text{idp}}}{N_{\varepsilon^2}} \sum_{N}^{i=1} \text{Re}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2 + \text{Im}[\tilde{\chi}_{\text{data}}(R_i) - \tilde{\chi}_{\text{theory}}(R_i)]^2)$$

And

$$r\chi^2 = \frac{\chi^2}{N_{\text{idp}} - N_{\text{var}}}$$

Where N_{idp} is the number of independent data points defined as $N_{\text{idp}} = \frac{(2\Delta r \Delta k)}{\pi}$, Δr is the fitting range in *r*-space, Δk is the fitting range in *k*-space, N_{ε^2} is the number of uncertainties to minimize, Re() is the real part of the EXAFS Fourier-transformed data and theory functions, Im() is the imaginary part of the EXAFS Fourier-transformed data and theory functions, and $\tilde{\chi}(R_i)$ is the Fourier-transformed data or theoretical function.

Additionally, IFEFFIT calculates the *R*-factor for each fit, which is directly proportional to χ^2 and is the root-mean-square difference between the data and calculated fit, and given by:

$$\boldsymbol{R} = \frac{\sum_{\text{i=1}}^{\text{n}} \{\text{Re}[\tilde{\chi}_{data}(\text{R}_\text{i}) - \tilde{\chi}_{theory}(\text{R}_\text{i})]^2 + \text{Im}[\tilde{\chi}_{data}(\text{R}_\text{i}) - \tilde{\chi}_{theory}(\text{R}_\text{i})]^2\}}{\sum_{\text{i=0}}^{\text{n}} \{\text{Re}[\tilde{\chi}_{data}(\text{R}_\text{i})]^2 + \text{Im}[\tilde{\chi}_{data}(\text{R}_\text{i})]^2\}}$$

C.3 Introduction

As mentioned in section 1.2, nickel is an inhibitor of the iron and α-ketoglutarate dependent dioxygenase family of enzymes which binds the active site iron via a His/His/Asp facial triad. PHD2 is inhibited by both Ni(II) and Zn(II), with Zn(II) having a greater inhibitory effect than Ni(II). The C201A mutation, which is on the surface of

PHD2, shows a different pattern of inhibition for Zn(II), leading to the hypothesis that Zn(II) is an allosteric inhibitor of PHD2. In order to test this hypothesis, XAS was performed to monitor the metal site structure of Ni(II) and Zn(II) in WT-PHD2 and C201A-PHD2.

C.4 Results

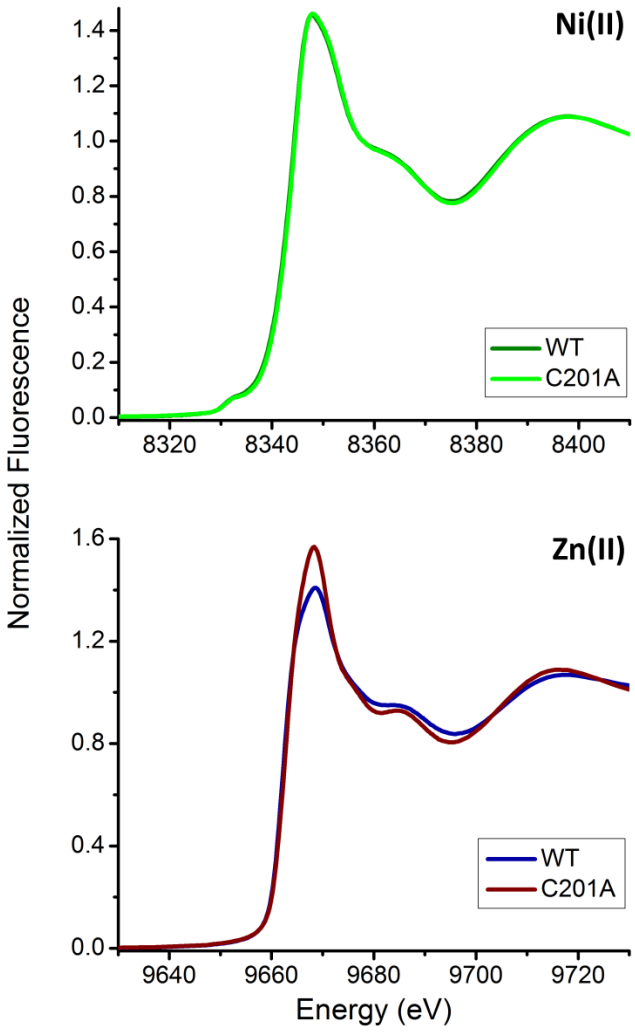

Figure C.1: XANES overlay of the metal complexes of WT- and C201A-PHD2 proteins in buffer with 50 mM PBS, 150 mM NaBr, pH 7.2: (Top) WT-PHD2 (green) and C201A-PHD2 (light green) with Ni(II); (Bottom) WT-PHD2 (blue) and C201A-PHD2 (wine) with Zn(II).

XANES Analysis

In the case of WT- and C201-PHD2 complexed to Ni(II) (**Figure C.1 Top**) the XANES region overlap completely, indicating that the mutation has not changed the coordination environment of the Ni(II) center in any way. Thus, Ni(II) does not appear to bind in the proposed allosteric site. Previous studies of Ni(II) have shown that Ni(II) inhibits non-home dioxygenases such as PHD2 by replacing iron in the active site (section 1.2). If this were indeed the case then Ni(II) coordination in the active site would theoretically be unchanged by the C201A mutation. Because the Ni(II) XANES spectra lack a $1s \rightarrow 4p_z$ transition a tetrahedral, four-coordinate, and square pyramidal geometries are not possible.[16] The $1s \rightarrow 3d$ transition has a large peak area (**Table C.1**), indicating that the Ni(II) centers do not have a centrosymmetric ligand arrangement.[16] Because the peak area is unnaturally large even for square-pyramidal complexes the Ni(II) spectra were proposed to be seven-coordinate complexes.

Zn(II) is a d^{10} metal and thus has no $1s \rightarrow 3d$ transitions. In addition, the $1s \rightarrow 4p_z$ transition occurs at such high energy that it is buried in the edge. Thus a more precise geometry cannot be determined through the XANES like it can with other transition metals. The spectra in **Figure C.2** are observably different, indicating a change in the first coordination sphere. However, because the normalized intensity of both spectra are between 1.3 – 1.8, both are five coordinate, although WT-PHD2 is in an ambiguous region.[17,18]

Table C.1: XAS Analysis for Metal Complexes of WT- and C201A-PHD2 Variants

in Buffer with 150 mM NaBr [a]

	XANES Analysis				EXAFS Analysis				
Sample	K-edge energy (eV)	1s → 3d peak area (x10^2 eV)	1s → $4p_z$ observed	Coordination #/geometry	Shell	*r* (Å)	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	%R
				WT-PHD2					
Ni(II)	8344.5	15(1)	No	7	5N/O	2.08(1)	1(1)	4(1)	3.1
					1S	2.51(1)	8(1)		
					1Br	2.46(1)	4(1)		
Zn(II)	9662.4	NA	NA	5	2N/O	2.09(2)	4(1)	-5(1)	1.4
					2S	2.31(1)	4(0)		
					1Imd	1.98(2)	5(2)		
				C201A-PHD2					
Ni(II)	8344.3	15(2)	No	7	5N/O	2.07(1)	2(1)	4(1)	3.2
					1S	2.50(1)	8(1)		
					1Br	2.45(1)	4(1)		
Zn(II)	9663.9	NA	NA	5	**1N/O**	**2.05(1)**	**5(1)**	**-5(1)**	**0.7**
					1S	**2.30(1)**	**3(1)**		
					1S	**2.44(1)**	**4(1)**		
					1Br	**2.38(2)**	**2(1)**		
					1Im 0°	**1.95(1)**	**1(1)**		
					3N/O	2.09(1)	2(1)	-5(1)	3.2
					1S	2.31(1)	2(1)		
					1Im 0°	1.96(1)	2(1)		

[a]The numbers in parentheses are the estimated uncertainties in the corresponding variables. These uncertainties are calculated by Artemis and reflect the change in the variable that will result in an increase in χ_2 of 1. EXAFS fits in bold type are shown in Figures C2-3.

EXAFS Analysis

EXAFS analysis of Ni(II) WT-PHD2 (**Table C.1** and **Figure C.2**) is consistent with a seven-coordinate site and the best fit features five N/O ligands, an S-donor ligand, presumably from the protein, and a bromide from solvent. The presence of a sulfur ligand indicates that the Ni(II) is bound to the protein but not in the active site. However, the lack of a second sulfur ligand lends doubt as to whether it is bound to the allosteric site, although the binding of two sulfur ligands may result in a change in spin state that is not supported by the ligand set available to the solvent exposed Ni(II). Because of data quality between 3 and 4 Å, contributions from multiple scattering could not be assessed.

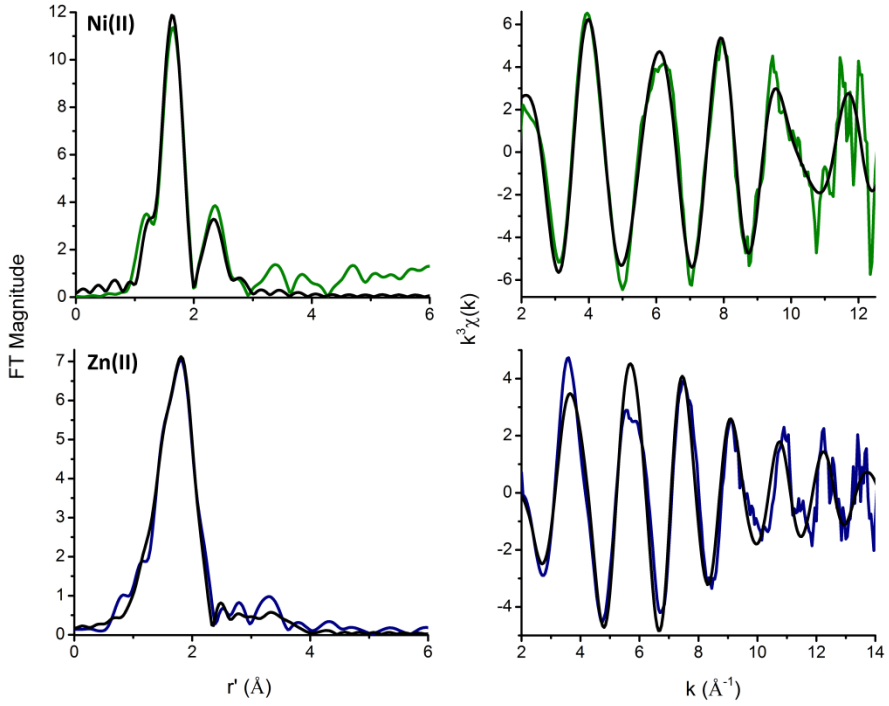

Figure C.2: *K*-edge XAS spectra of WT-PHD2 metal complexes with Ni(II) (Top) and Zn(II) (Bottom) in buffer with 50 mM PBS, 150 mM NaBr, pH 7.2. Left: Fourier filtered XAS data (colored lines) and best fits (black lines). Right: Unfiltered *k*3-weighted EXAFS spectra (colored lines) and fits (black).

EXAFS analysis of Ni(II) C201A-PHD2 reveals an identical coordination sphere as Ni(II) WT-PHD2, which is expected when considering the identical XANES spectrum. The best fit consists of 5 N/O ligands, one sulfur ligand and one bromide from solvent, all at distances identical to Ni(II) WT-PHD2. Again, the presence of a sulfur indicates that the Ni(II) is not binding in the active site but is binding to the protein in some fashion, as these samples were prepared in buffer with NaBr. While it is not clear if Ni(II) is binding to the proposed allosteric site, what is clear is that the mutated cysteine is not involved in Ni(II) coordination. If Ni(II) is in the allosteric site but is not binding to C201, this would indicate that C208 is somehow a more favorable ligand because of their close proximity. If this hypothesis is true, mutation of C208 should give a different XANES and EXAFS spectrum for Ni(II).

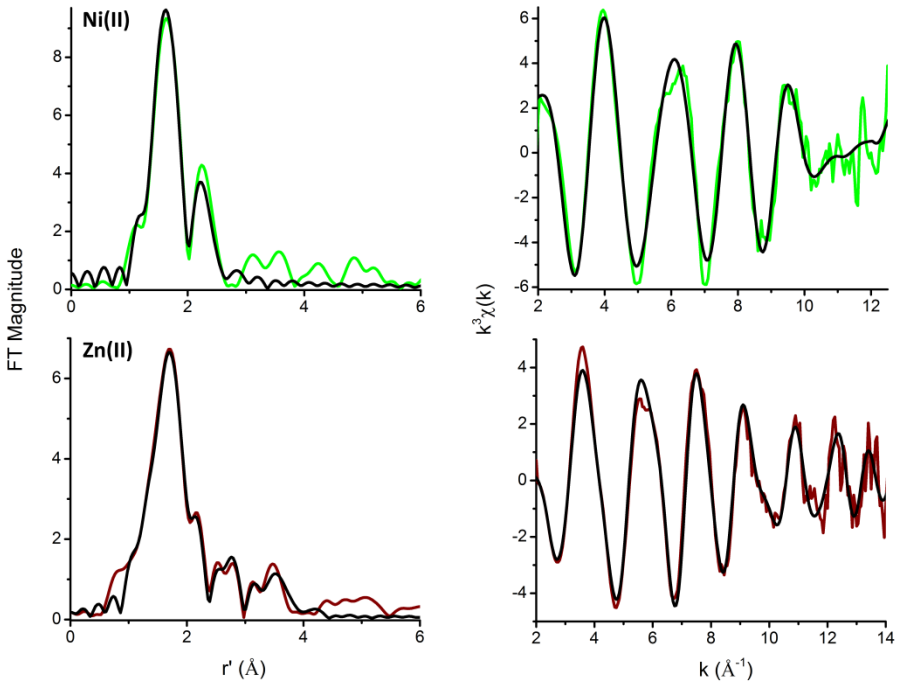

Figure C.3: *K*-edge XAS spectra of C201A-PHD2 metal complexes with Ni(II) (Top) and Zn(II) (Bottom) in buffer with 50 mM PBS, 150 mM NaBr, pH 7.2. Left: Fourier filtered XAS data (colored lines) and best fits (black lines). Right: Unfiltered *k*3-weighted EXAFS spectra (colored lines) and fits (black).

EXAFS analysis of Zn(II) WT-PHD2 is consistent with a five-coordinate geometry, corresponding with the XANES analysis. The best fit consists of two N/O ligands, two sulfur ligands and an imidazole. The presence of two sulfur ligands precludes Zn(II) binding to the active site. The proposed allosteric site of PHD2 is the only place where two sulfur ligands are in close enough proximity that both could act as ligands to Zn(II). As Zn(II) is a d^{10} metal a change in spin state is not a factor in binding to both sulfur ligands. The presence of an imidazole is possible, as His205 is immediately adjacent to both Zn(II) ligands. The lack of a bromide from solvent despite the obvious solvent accessibility is understandable because binding of both cysteines, assuming deprotonation, would result in a charge neutral complex, thus favoring water binding instead of bromide.

Zn(II) C201A-PHD2 is perhaps the most ambiguous of all the results, as the best fit is clearly consistent with one N/O ligands, two sulfur ligands, a bromide from solvent and an imidazole ligand. However, the sulfur distances are not far enough apart to split given the resolution of the data set. The next best fit, while significantly worse, is five coordinate with three N/O ligands, one sulfur and an imidazole ligand. This fit also correlates with the change seen in the XANES spectrum, as the intensity increased but the coordination remained the same, which is indicative of the loss of a sulfur ligand.[18] What is clear is that the C201A mutation affects the Zn(II) structure, implicating it as a Zn(II) ligand and indicating that inhibition of PHD2 by Zn(II) occurs at an allosteric site.

APPENDIX D

NISOD OXIDIZED WITH $IrCl_6$

D.1 Experimental Procedures

D.1.1 Cloning and Mutagenasis

All the data in this section were handled as outlined in Chapter 7, Section 7.2.1.

D.1.2 NiSOD Expression and Purification

All the data in this section were handled as outlined in Chapter 7, Section 7.2.2.

D.1.3 Metallation of NiSOD

All the data in this section were handled as outlined in Chapter 7, Section 7.2.3.

D.1.4 UV-Vis Spectroscopy

All the data in this section were handled as outlined in Chapter 7, Section 7.2.7.

D.1.5 X-ray Absorption Spectroscopy

All the data in this section were handled as outlined in Chapter 7, Section 7.2.9.

D.1.6 Data Reduction and Analysis

All the data in this section were handled as outlined in Chapter 7, Section 7.2.10.

D.2 Results

D.2.1 UV-Vis Spectroscopy

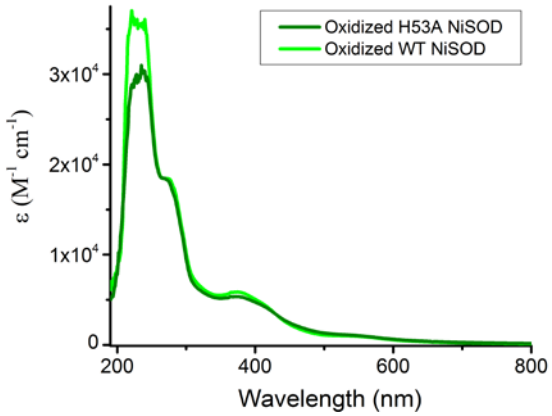

Figure D.1: UV-Vis spectra of $IrCl_6$ oxidized WT- and H53A-NiSOD.

The purpose of mutating H53A-NiSOD was to disrupt any possible cross talk between nickel centers that may allow for maintaining a half Ni(II) half Ni(III) state for the hexamer. The UV-Vis spectra of IrCl6 oxidized WT- and H53A-NiSOD displays no difference between these two mutations, indicating that H53A-NiSOD does not have a higher Ni(III)/Ni(II) ratio that WT-NiSOD. This would mean that the ion bridge in which H53 is involved in is not responsible for redox state maintenance.

D2.2 XANES Analysis

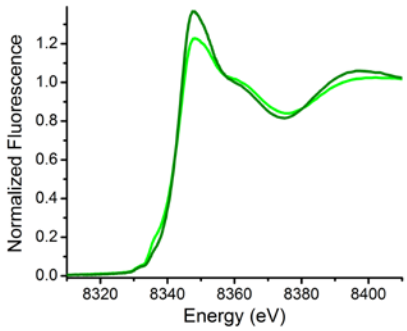

Figure D.2: *K*-edge XAS spectra of $IrCl_6$ oxidized WT- (light green) and H53A-NiSOD (dark green) with Ni(II) in buffer containing 20 mM Tris, 100 mM NaCl, and 10% glycerol at pH 8.0.

XANES (X-ray absorption near edge structure) analysis can yield information on coordination number and geometry of the metal site. Nickel has vacancies in its 3d orbitals, allowing for a transition whose intensity is dependent on the coordination number and geometry. Centrosymmetric geometries (four-coordinate planar, six-coordinate octahedral) produce smaller 1s → 3d transitions than non-centrosymmetric (tetrahedral, four-coordinate pyramidal).[16] The 1s → $4p_z$ transition (plus shakedown) occurs when one or both axial positions are unoccupied which can thus allow differentiation between geometries with similar 1s → 3d transitions (four-coordinate planar v. six-coordinate octahedral).[16] Both of these transitions are observed in the XANES spectrum of $IrCl_6$ oxidized WT- and H53A-NiSOD.

The XANES of oxidized WT-NiSOD has a larger 1s → 3d than the reduced sample which is expected, as oxidized WT-NiSOD is a mixture of four-coordinate planar and four-coordinate pyramidal geometries. The 1s → $4p_z$ transition is anticipated to decrease as there is now significant four-coordinate pyramidal character, which has one axial ligand and thus a less intense transition, and the XANES reflects this. The XANES of oxidized H53A-NiSOD has a smaller 1s → 3d than the reduced sample but which remains on the border of four-coordinate pyramidal and planar geometries.[16] The 1s → $4p_z$ is much smaller than in WT-NiSOD indicating that the mixture in H53A-NiSOD has more axial ligand bound. This is not supported by EPR or UV-Vis which indicates that this is purely a structural change and has no relation to the oxidation state. The EPR and UV-Vis maintains an ~50% Ni(III) species and no change in the contribution of the g_z signal, possibly indicating that this increase in axial character is attributed to the Ni(II) species.

D2.3 EXAFS Analysis

Table D.1: XANES and EXAFS Analysis for Oxidized Metal Complexes of WT- and H53A-NiSOD in 20 mM Tris, 100 mM NaCl, 10% glycerol, pH 8.0.

	XANES Analysis				EXAFS Analysis					
Sample	K-edge energy (eV)	1s → 3d peak area (x10^2 eV)	1s → $4p_z$ observed	Coord #/geometry	Shell	*r* (Å)	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	%R	rχ^2
				WT-NiSOD						
Ox Ni(II)	8334.7	6.2(5)	Yes	5/pyramidal	1 N/O	1.90(2)	1(4)	-3(3)	3.4	16
					1 N/O	2.07(6)	3(26)			
					1 S	2.31(3)	6(3)			
					1 S	2.18(2)	4(4)			
					4 C	2.93(6)	3(1)			
					1 N/O	**1.90(1)**	**1(1)**	**-3(1)**	**1.4**	**8.0**
					1 N/O	**2.17(1)**	**6(1)**			
					1 S	**2.31(2)**	**3(2)**			
					1 S	**2.17(1)**	**4(1)**			
					3 C	**2.90(3)**	**10(4)**			
					0.5 Imd	**2.01(1)**	**2(1)**			
					1 N/O	1.90(1)	7(1)	-4(1)	0.85	6.1
					1 N/O	2.16(1)	0(1)			
					1 S	2.30(1)	1(1)			
					1 S	2.16(1)	5(1)			
					3 C	2.89(2)	13(3)			
					1 Cl	3.53(3)	10(4)			
					0.5 Imd	2.00(2)	1(1)			
					1 N/O	1.90(1)	0(1)	-2(1)	1.6	8.8
					1 N/O	2.16(2)	5(2)			
					1 S	2.31(2)	4(2)			
					1 S	2.17(1)	3(1)			
					3 C	2.89(3)	9(4)			
					1 Imd	2.01(2)	2(1)			
				H53A-NiSOD						
Ox Ni(II)	8335.3	4.3(8)	Yes	5/pyramidal	1 N/O	1.95(1)	3(1)	-2(2)	3.5	12.5
					1 N/O	2.07(1)	5(1)			
					1 S	2.25(4)	4(4)			
					1 S	2.39(8)	12(12)			
					2 C	2.95(4)	11(5)			
					1 N/O	**1.93(2)**	**1(2)**	**-2(2)**	**2.7**	**11.6**
					1 N/O	**2.07(1)**	**4(1)**			
					1 S	**2.38(5)**	**7(8)**			
					1 S	**2.23(4)**	**4(6)**			
					4 C	**2.92(4)**	**9(4)**			
					0.7 Imd	**2.02(3)**	**1(3)**			
					1 N/O	1.95(2)	2(2)	-1(2)	2.6	11.3
					1 N/O	2.08(1)	4(1)			
					1 S	2.39(20)	22(35)			
					1 S	2.27(6)	9(6)			
					4 C	2.93(4)	10(5)			
					1 Imd	2.04(4)	4(4)			

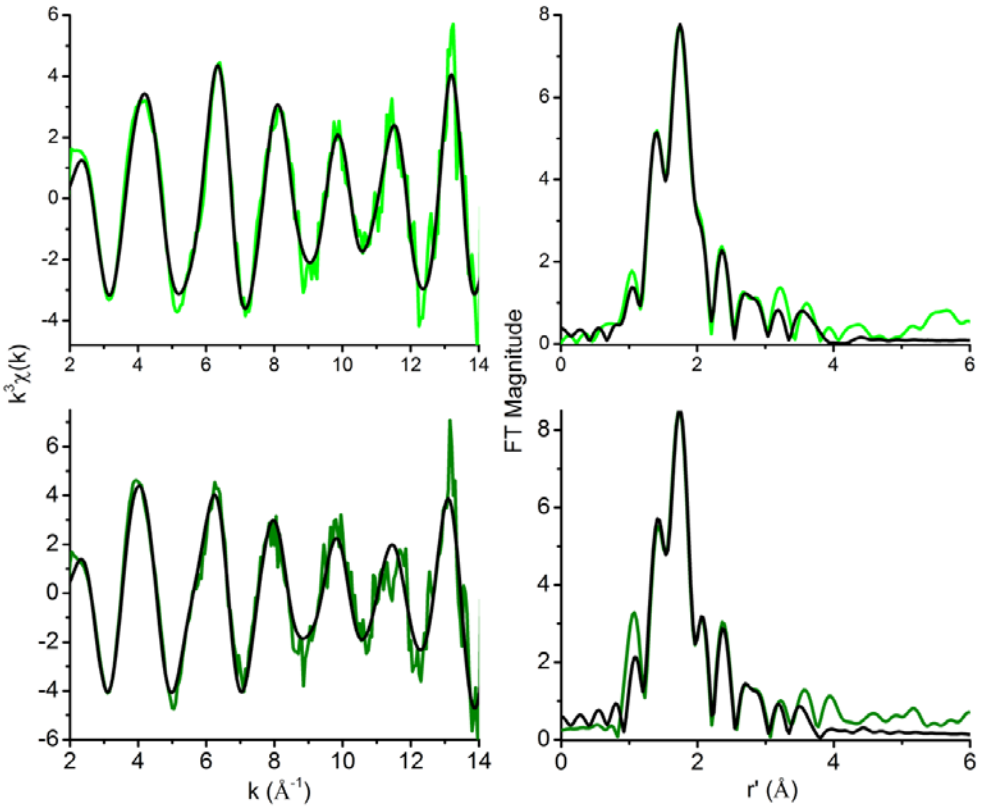

Figure D.3: *K*-Edge XAS spectra of $IrCl_6$ oxidized WT- (Top) and H53A-NiSOD (Bottom) metal complexes in buffer containing 20 mM Tris, 100 mM NaCl, 10% glycerol at pH 8.0: (Left) Unfiltered k^3-weighted EXAFS spectra (colored lines) and fits (black lines). (Right) Fourier-transformed EXAFS data and fits.

The EXAFS (extended x-ray absorption fine structure) region of the XAS spectrum can provide information on the number and type of scattering atoms and their distance from the absorbing atom which in this case is nickel. The EXAFS of WT-NiSOD was fit in order to allow comparison with the mutant at equal *r*- and *k*-range, as well as to assess the change in fitting method. The best fit for the oxidized WT-NiSOD spectrum has elongated Ni-S distances (See Chapter 2), as expected of a change from four-coordinate planar to pyramidal geometry. In addition, both chlorides are gone and are instead replaced by ~0.5 imidazole ligands, consistent with previous analysis indicating an approximately equal mixture of the two geometries in the oxidized enzyme.

The best fit of the oxidized H53A-NiSOD EXAFS spectrum is again nearly identical to that of WT-NiSOD, lacking both chlorides but with ~0.7 imidazoles instead of ~0.5. This is consistent with XANES analysis, but not that of EPR or UV-Vis, again indicating a structural change that is not correlated to an electronic change.

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APPENDIX E

ADDITIONAL FIT TABLES FOR WT RCNR

Table E.1. Additional Fits for Ni(II) WT-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(1)	1(1)	3(4)	0.2713	2567.560	130.733	3
3N/O	2.07(1)	3(1)	3(2)	0.1899	1797.211	91.509	3
4N/O	2.07(1)	4(1)	2(2)	0.1654	1565.177	79.695	3
5N/O	2.07(1)	6(1)	2(2)	0.1749	1655.572	84.297	3
6N/O	2.07(1)	7(1)	1(2)	0.2039	1930.141	98.278	3
7N/O	2.07(2)	9(1)	1(2)	0.2425	2295.086	116.860	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.16(2)	5(1)	-19(5)	0.2764	2616.280	133.214	3
3S	2.16(2)	7(1)	-19(4)	0.2491	2357.763	120.051	3
4S	2.16(2)	9(1)	-19(4)	0.2524	2388.674	121.625	3
5S	2.17(2)	12(1)	-19(4)	0.2674	2531.159	128.880	3
6S	2.17(3)	13(1)	-20(4)	0.2865	2712.154	138.096	3
7S	2.17(3)	15(2)	-20(4)	0.3064	2900.279	147.675	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.04(2)	0(2)					
1N/O	2.15(3)	1(3)	3(3)	0.1768	1673.369	94.864	5
2N/O	2.05(4)	2(2)					
2N/O	2.11(7)	6(8)	2(3)	0.1625	1537.991	87.189	5
3N/O	2.06(2)	3(2)					
1N/O	2.16(8)	4(10)	3(3)	0.1618	1531.471	86.820	5
4N/O	2.07(1)	4(1)					
1N/O	2.31(0.11)	14(23)	4(2)	0.1569	1484.604	84.163	5
3N/O	2.07(1)	3(1)					
2N/O	2.20(0.13)	20(19)	4(3)	0.1589	1503.894	85.256	5
5N/O	2.08(1)	6(1)					
1N/O	2.37(8)	9(11)	4(2)	0.1610	1523.760	86.383	5

4N/O	2.08(1)	4(1)					
2N/O	2.33(7)	17(14)	5(2)	0.1524	1442.924	81.800	5
3N/O	2.07(1)	3(1)					
3N/O	2.25(0.10)	26(18)	5(3)	0.1566	1481.879	84.008	5
6N/O	2.08(1)	7(1)					
1N/O	2.39(6)	7(8)	3(2)	0.1801	1705.043	96.660	5
5N/O	2.08(1)	5(1)					
2N/O	2.37(5)	12(9)	5(2)	0.1568	1483.880	84.122	5
4N/O	2.08(1)	4(1)					
3N/O	2.34(6)	20(11)	6(2)	0.1518	1437.162	81.473	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.15(2)	3(1)					
1S	2.29(4)	4(4)	-15(5)	0.2263	2141.593	121.408	5
2S	2.16(2)	4(2)					
2S	2.30(5)	11(6)	-14(5)	0.2163	2047.681	116.084	5
3S	2.17(2)	6(1)					
1S	2.34(4)	5(4)	-15(4)	0.2201	2083.357	118.106	5
4S	2.14(2)	7(1)					
1S	1.94(4)	8(5)	-26(5)	0.2333	2208.626	125.208	5
3S	2.17(2)	6(1)					
2S	2.35(5)	12(6)	-13(4)	0.2117	2003.989	113.607	5
5S	2.17(2)	12(1)					
1S	2.87(3)	3(2)	-19(3)	0.1884	1783.152	101.088	5
4S	2.19(2)	8(1)					
2S	2.40(4)	11(5)	-13(4)	0.2107	1993.938	113.037	5
3S	2.18(2)	7(1)					
3S	2.37(4)	16(6)	-12(4)	0.2010	1902.862	107.874	5
6S	2.13(2)	10(1)					
1S	1.90(2)	6(2)	-27(5)	0.2247	2126.887	120.574	5
5S	2.20(2)	10(1)					
2S	2.43(4)	10(5)	-13(4)	0.2130	2015.821	114.278	5
4S	2.19(2)	8(1)					
3S	2.41(4)	14(5)	-11(3)	0.1989	1882.257	106.706	5

Ni-N(2.0) Ni-S(2.2)							
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.04(2)	1(1)					5
1S	2.26(4)	7(4)	-2(4)	0.2245	2125.090	120.472	
1N/O	1.85(0.11)	10(13)					5
2S	2.15(2)	5(1)	-21(6)	0.2566	2428.258	137.659	
2N/O	1.86(0.11)	15(14)					
2S	2.15(2)	5(1)	-21(7)	0.2496	2362.381	133.924	5
3N/O	2.08(1)	3(1)					
1S	2.62(2)	6(3)	5(2)	0.1359	1286.627	72.939	5
1N/O	1.78(4)	6(5)					
3S	2.15(2)	7(1)	-23(4)	0.2307	2183.931	123.808	5
1N/O	2.25(3)	1(2)					
4S	2.19(2)	8(1)	-17(5)	0.2287	2164.487	122.706	5
4N/O	2.18(1)	4(1)					
1S	2.62(2)	6(2)	4(1)	0.1060	1002.910	56.855	5
2N/O	2.72(3)	2(3)					
3S	2.18(2)	8(1)	-15(4)	0.2108	1995.556	113.129	5
3N/O	2.08(1)	3(1)					
2S	2.61(3)	15(5)	5(2)	0.1393	1318.214	74.730	5
5N/O	2.07(1)	5(1)					
1S	2.00(0.11)	21(18)	4(3)	0.1652	1563.630	88.643	5
1N/O	2.26(3)	1(2)					
5S	2.19(2)	11(1)	-17(4)	0.2276	2153.859	122.103	5
4N/O	2.08(1)	4(1)					
2S	2.61(3)	13(3)	5(1)	0.1078	1020.276	57.840	5
2N/O	2.72(3)	2(2)					
4S	2.19(2)	10(1)	-15(4)	0.2005	1897.976	107.597	5
3N/O	1.80(7)	18(12)					
3S	2.15(2)	7(1)	-23(5)	0.2329	2204.227	124.959	5
6N/O	2.07(2)	5(2)					
1S	2.03(9)	10(8)	2(2)	0.1660	1571.233	89.074	5
1N/O	2.27(2)	1(2)	-17(4)	0.2342	2216.703	125.666	5

6S	2.20(3)	13(2)					
5N/O	2.07(1)	6(1)					
2S	1.98(6)	29(15)	5(2)	0.1621	1533.832	86.954	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.80(8)	22(15)					
3S	2.15(2)	7(1)	-23(5)	0.2326	2201.950	124.830	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	11(2)					
1Imd	2.05(2)	1(1)	3(2)	0.1440	1157.916	65.643	5
4N/O	2.08(2)	5(2)					
1Imd	1.88(4)	5(4)					
1Imd	2.03(3)	1(2)	-1(2)	0.1093	1034.944	66.174	7
3N/O	2.08(2)	4(2)					
1Imd	2.11(3)	2(3)					
1Imd	1.99(3)	3(3)					
1Imd	1.86(3)	0(3)	-1(2)	0.0969	917.509	67.268	9
2N/O	2.08(2)	2(2)					
1Imd	2.01(4)	4(4)					
1Imd	2.13(4)	3(5)					
1Imd	2.23(0.35)	25(102)					
1Imd	1.89(5)	1(5)	1(4)	0.1075	1017.790	87.442	11
1N/O	2.07(2)	1(2)					
1Imd	2.12(6)	11(3)					
1Imd	2.39(0.10)	2(12)					
1Imd	1.91(6)	4(4)					
1Imd	2.01(6)	10(3)					
1Imd	2.23(7)	9(4)	3(3)	0.1157	1095.568	113.652	13
4N/O	2.09(2)	7(2)					
1Imd	2.05(2)	1(2)	3(2)	0.1306	1235.739	70.055	5
3N/O	2.08(2)	4(2)					
1Imd	2.04(3)	2(3)					
1Imd	1.93(5)	8(9)	1(2)	0.1158	1095.913	70.073	7
2N/O	2.08(2)	2(2)	0(2)	0.1087	1029.012	75.443	9

1Imd	1.89(3)	1(4)					
1Imd	2.13(3)	3(3)					
1Imd	2.01(3)	4(3)					
1N/O	2.07(2)	1(2)					
1Imd	2.09(3)	9(3)					
1Imd	1.98(3)	9(3)					
1Imd	2.19(3)	7(3)					
1Imd	1.87(4)	3(3)	1(2)	0.1273	1204.464	103.479	11
0N/O							
1Imd	2.19(5)	9(8)					
1Imd	2.27(0.19)	7(40)					
1Imd	1.99(5)	10(6)					
1Imd	1.90(6)	4(7)					
1Imd	2.09(5)	11(7)	3(3)	0.2168	2051.559	176.256	11
3N/O	2.09(2)	4(2)					
1Imd	2.04(3)	2(3)	3(2)	0.1291	1221.614	69.254	5
2N/O	2.08(2)	2(2)					
1Imd	2.13(6)	4(7)					
1Imd	2.01(4)	2(3)	3(2)	0.1315	1244.367	79.565	7
1N/O	2.08(3)	0(2)					
1Imd	2.15(3)	3(4)					
1Imd	1.94(6)	2(7)					
1Imd	2.03(3)	4(4)	2(2)	0.1446	1369.073	100.374	9
0N/O							
1Imd	1.91(4)	3(6)					
1Imd	2.19(4)	7(5)					
1Imd	2.00(4)	9(4)					
1Imd	2.10(4)	9(4)	2(2)	0.2258	2137.088	156.682	9
2N/O	2.08(2)	2(2)					
1Imd	2.04(4)	2(3)	3(2)	0.1620	1533.055	86.910	5
1N/O	2.08(2)	0(2)					
1Imd	2.02(3)	1(2)					
1Imd	2.14(3)	0(3)	4(2)	0.1695	1604.535	102.594	7
0N/O							
1Imd	2.16(3)	5(4)					
1Imd	2.05(4)	5(4)					
1Imd	1.97(6)	1(8)	3(2)	0.2480	2347.496	150.099	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**

4N/O	2.09(3)	7(3)					
1S	1.96(0.15)	32(42)					
1Imd	2.05(3)	2(2)	4(2)	0.1261	1193.515	76.313	7
3N/O	2.08(2)	4(2)					
1S	1.84(0.11)	27(20)					
1Imd	1.90(7)	7(7)					
1Imd	2.04(3)	1(3)	2(2)	0.1101	1041.848	76.384	9
2N/O	2.09(2)	2(2)					
1S	2.62(2)	5(2)					
1Imd	2.12(5)	0(8)					
1Imd	2.01(4)	0(6)					
1Imd	2.24(6)	2(9)	6(2)	0.0582	550.636	47.307	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(3)	7(3)					
1S	1.97(0.13)	20(37)					
1Imd	2.05(3)	2(2)	4(2)	0.1254	1186.558	75.869	7
3N/O	2.09(1)	5(2)					
1S	2.62(2)	6(2)					
1Imd	2.05(2)	1(1)					
1Imd	2.18(5)	7(7)	5(1)	0.0503	746.249	34.917	9
2N/O	2.08(2)	2(2)					
1S	2.62(2)	5(2)					
1Imd	2.02(0.35)	3(29)					
1Imd	2.09(0.31)	3(41)					
1Imd	2.22(0.10)	4(16)	5(2)	0.0552	522.662	44.904	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(1)	8(1)					
1S	2.62(2)	6(2)					
1Imd	2.05(1)	1(1)	4(1)	0.053	501.976	32.096	7
3N/O	2.09(1)	5(2)					
1S	2.63(2)	6(2)					
1Imd	2.05(2)	1(2)					
1Imd	2.18(5)	8(7)	5(1)	0.0484	457.785	33.563	9
2N/O	2.08(1)	2(2)					
1S	2.62(2)	6(2)					
1Imd	2.21(0.10)	4(14)					
1Imd	2.04(0.52)	6(49)					
1Imd	2.06(0.40)	3(10)	5(2)	0.0531	502.491	43.171	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(1)	8(1)					
1S	2.62(1)	6(2)					
1Imd	2.05(1)	1(1)	4(1)	0.0513	485.581	31.048	7
3N/O	2.09(1)	5(2)					
1S	2.63(2)	6(2)					
1Imd	2.18(5)	8(7)					
1Imd	2.05(2)	1(2)	5(1)	0.0469	444.245	32.570	9
2N/O	2.08(1)	2(2)					
1S	2.62(2)	6(2)					
1Imd	2.02(0.31)	6(35)					
1Imd	2.06(0.23)	2(8)					
1Imd	2.21(8)	3(11)	4(2)	0.0514	486.881	41.830	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(1)	8(1)					
1S	2.63(1)	6(2)					
1Imd	2.05(1)	1(1)	4(1)	0.0499	472.106	30.187	7
3N/O	2.09(1)	5(2)					
1S	2.63(1)	6(2)					
1Imd	2.17(5)	8(8)					
1Imd	2.04(2)	2(2)	5(1)	0.0456	431.668	31.648	9
3N/O	2.09(1)	5(2)					
1S	2.63(1)	6(2)					
1Imd 0o	2.05(2)	2(2)					
1Imd 5o	2.19(4)	7(6)	5(1)	0.0461	436.280	31.986	9
3N/O	2.11(2)	7(3)					
1S	2.62(2)	6(2)					
1Imd 0o	2.06(2)	2(1)					
1Imd 10o	2.04(5)	5(3)	4(1)	0.0442	418.444	30.678	9
3N/O	2.10(2)	8(3)					
1S	2.62(2)	6(2)					
1Imd 05o	2.06(2)	1(1)					
1Imd 10o	2.05(6)	6(6)	4(1)	0.0502	475.207	34.840	9
2N/O	2.08(1)	2(1)					
1S	2.62(2)	5(2)					
1Imd	2.02(0.26)	6(32)					
1Imd	2.20(7)	3(11)					
1Imd	2.06(0.18)	2(7)	4(2)	0.0499	472.104	40.560	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	2(2)					
1N/O	2.21(6)	7(11)					
1S	2.63(2)	5(2)					
1Imd 0o	2.13(9)	6(14)					
1Imd 0o	2.03(7)	3(7)	5(1)	0.0405	382.917	32.898	11
2N/O	2.08(2)	2(2)					
1N/O	2.24(5)	5(8)					
1S	2.63(2)	5(2)					
1Imd 0o	2.13(4)	2(5)					
1Imd 5o	2.02(4)	1(4)	5(1)	0.0406	383.940	32.986	11
2N/O	2.07(2)	2(2)					
1N/O	2.21(3)	3(4)					
1S	2.63(2)	6(2)					
1Imd 0o	2.07(3)	3(2)					
1Imd 10o	2.02(6)	6(5)	4(1)	0.0381	360.950	31.010	11
2N/O	2.07(2)	2(2)					
1N/O	2.21(4)	4(6)					
1S	2.63(2)	6(2)					
1Imd 5o	2.08(3)	3(3)					
1Imd 10o	2.05(8)	7(8)	4(1)	0.0445	421.170	36.184	11
1N/O	2.07(3)	0(2)					
2N/O	2.14(4)	10(8)					
1S	2.63(2)	5(2)					
1Imd 0o	2.12(0.10)	6(17)					
1Imd 0o	2.03(9)	3(7)	4(1)	0.0406	383.995	32.990	11
1N/O	2.06(3)	1(2)					
2N/O	2.14(5)	9(9)					
1S	2.63(2)	6(2)					
1Imd 0o	2.06(6)	4(5)					
1Imd 5o	2.09(0.19)	10(20)	4(1)	0.0422	399.215	34.298	11
1N/O	2.06(3)	1(2)					
2N/O	2.15(3)	8(6)					
1S	2.62(2)	6(2)					
1Imd 0o	2.07(2)	3(2)					
1Imd 10o	2.02(6)	6(5)	3(1)	0.0377	356.576	30.635	11

1N/O	2.06(3)	1(2)					
2N/O	2.15(4)	9(7)					
1S	2.62(2)	6(2)					
1Imd 5o	2.07(3)	3(3)					
1Imd 10o	2.05(8)	7(7)	4(1)	0.0441	417.198	35.843	11

Table E.2. Additional Fits for Co(II) WT-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.12(3)	5(2)	5(4)	0.3687	739.168	44.004	3
3N/O	2.11(3)	7(2)	3(3)	0.2715	588.738	35.048	3
4N/O	2.10(2)	10(2)	2(3)	0.2255	488.838	29.101	3
5N/O	2.10(2)	12(2)	1(2)	0.2092	453.594	27.003	3
6N/O	2.09(2)	14(2)	0(2)	0.2102	455.723	27.130	3
7N/O	2.09(3)	16(2)	-1(3)	0.2207	478.559	28.489	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.23(3)	9(2)	-13(6)	0.3272	709.308	42.226	3
3S	2.23(3)	12(2)	-14(5)	0.2561	555.271	33.056	3
4S	2.22(3)	15(2)	-15(4)	0.2207	478.578	28.490	3
5S	2.22(3)	17(2)	-16(4)	0.2039	442.083	26.318	3
6S	2.22(3)	19(2)	-17(4)	0.1974	428.046	25.482	3
7S	2.21(3)	20(2)	-18(4)	0.1970	427.067	25.424	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.03(2)	1(1)					
1N/O	2.18(1)	3(1)	1(2)	0.1517	328.987	22.232	5
2N/O	2.00(2)	2(1)					
2N/O	2.16(2)	1(1)	-1(2)	0.1456	315.781	21.340	5
3N/O	2.04(2)	5(1)					
1N/O	2.18(1)	2(1)	-1(2)	0.1369	296.841	20.060	5
4N/O	2.04(2)	8(2)					
1N/O	2.18(2)	1(1)	-2(2)	0.1457	315.975	21.353	5
3N/O	2.01(2)	5(2)					
2N/O	2.16(2)	2(1)	-2(2)	0.1577	341.980	23.110	5
5N/O	2.04(2)	11(2)					
1N/O	2.17(2)	0(2)	-3(2)	0.1648	357.347	24.149	5

4N/O	2.01(2)	9(2)					
2N/O	2.16(2)	3(2)	-3(2)	0.1791	388.203	26.234	5
3N/O	1.98(3)	7(3)					
3N/O	2.14(2)	5(2)	-3(2)	0.1909	413.990	27.976	5
6N/O	2.03(2)	13(2)					
1N/O	2.17(2)	1(2)	-4(2)	0.1870	405.414	27.397	5
5N/O	2.01(3)	12(3)					
2N/O	2.15(3)	4(3)	-4(3)	0.2013	436.418	29.492	5
4N/O	1.99(4)	12(4)					
3N/O	2.14(3)	6(3)	-4(3)	0.2122	460.010	31.086	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.13(3)	7(2)					
1S	2.27(2)	2(1)	-20(4)	0.1893	410.390	27.733	5
2S	2.10(3)	7(2)					
2S	2.25(2)	5(2)	-20(4)	0.1731	375.372	25.367	5
3S	2.14(3)	10(2)					
1S	2.27(2)	3(2)	-21(4)	0.1735	376.158	25.420	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.24(3)	7(2)					
2S	2.08(3)	8(2)	-21(4)	0.1749	379.132	25.621	5
5S	2.23(2)	17(2)					
1S	3.07(6)	9(6)	-15(3)	0.1734	375.944	25.405	5
4S	2.23(2)	14(2)					
2S	3.08(6)	16(8)	-14(3)	0.1821	394.816	26.681	5
3S	2.25(3)	8(2)					
3S	2.09(3)	11(3)	-22(4)	0.1788	387.649	26.196	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.23(4)	18(3)					
2S	1.68(0.16)	42(20)	-14(6)	0.1921	416.443	28.142	5
4S	2.24(3)	11(3)	-22(5)	0.1849	400.783	27.084	5

3S	2.08(4)	13(4)					

Co-N(2.0) Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	5(2)					5
1S	2.28(2)	3(1)	-9(3)	0.1688	366.079	24.739	
1N/O	1.95(3)	2(2)					5
2S	2.25(2)	8(1)	-12(4)	0.1793	388.674	26.266	
2N/O	1.96(3)	7(3)					
2S	2.26(2)	8(2)	-12(4)	0.1683	364.869	24.657	5
3N/O	2.00(3)	8(2)					
1S	2.28(2)	4(1)	-8(3)	0.1555	337.078	22.779	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.00(4)	12(3)					
1S	2.28(2)	5(2)	-8(4)	0.1547	335.438	22.668	5
2N/O	1.94(5)	10(4)					
3S	2.25(3)	12(2)	-14(4)	0.1775	384.798	26.004	5
3N/O	1.97(5)	11(3)					
2S	2.27(3)	9(2)	-11(4)	0.1697	367.928	24.864	5
5N/O	2.01(4)	15(3)					
1S	2.28(2)	6(2)	-8(4)	0.1582	342.931	23.174	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.98(6)	16(4)					
2S	2.26(3)	10(3)	-11(5)	0.1728	374.688	25.320	5
2N/O	2.76(0.10)	14(15)					
4S	2.24(3)	14(2)	-13(4)	0.2035	441.121	29.810	5
3N/O	1.96(8)	15(6)					
3S	2.25(3)	13(3)	-13(6)	0.1807	391.851	26.480	5
6N/O	2.03(6)	19(3)					
1S	2.28(2)	7(3)	-7(5)	0.1623	351.955	23.784	5

1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.01(9)	20(5)					
2S	2.26(3)	11(3)	-10(6)	0.1749	379.281	25.631	5
2N/O	1.94(0.22)	21(15)					
5S	2.23(4)	18(4)	-16(7)	0.1909	413.978	27.976	5
4N/O	1.98(0.12)	21(7)					
3S	2.25(4)	14(4)	-12(7)	0.1824	395.389	26.719	5
3N/O	1.96(0.16)	21(10)					
4S	2.24(4)	16(4)	-14(7)	0.1873	406.054	27.440	5

Co-N(2.0) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(3)	15(3)					
1Imd	2.13(4)	6(4)	0(2)	0.1498	300.393	20.300	5
4N/O	2.06(3)	18(4)					
1Imd	2.02(1)	1(1)					
1Imd	2.16(1)	2(1)	-1(1)	0.0635	137.746	10.763	7
3N/O	2.07(3)	16(5)					
1Imd	1.93(4)	2(5)					
1Imd	2.04(2)	3(3)					
1Imd	2.17(2)	4(2)	-3(1)	0.0500	108.393	10.038	9
2N/O	2.08(3)	11(6)					
1Imd	1.86(4)	1(5)					
1Imd	1.96(3)	8(4)					
1Imd	2.19(2)	8(3)					
1Imd	2.07(3)	10(3)	-4(1)	0.0486	105.411	11.981	11
1N/O	2.07(5)	6(6)					
1Imd	2.27(5)	9(6)					
1Imd	2.06(4)	17(3)					
1Imd	1.85(4)	7(3)					
1Imd	1.95(4)	15(3)					
1Imd	2.17(4)	15(4)	-3(2)	0.0477	103.420	15.214	13
4N/O	2.07(3)	12(3)					
1Imd	2.15(4)	5(3)	0(2)	0.1532	332.185	22.448	5
3N/O	2.06(3)	14(4)					
1Imd	2.02(2)	0(2)					
1Imd	2.17(1)	2(1)	-1(1)	0.0661	143.214	11.190	7

2N/O	2.07(3)	11(5)					
1Imd	1.94(3)	1(4)					
1Imd	2.05(2)	4(3)					
1Imd	2.17(2)	4(2)	-2(1)	0.0534	115.782	10.723	9
1N/O	2.09(4)	5(5)					
1Imd	2.19(2)	8(2)					
1Imd	1.97(3)	10(3)					
1Imd	2.08(3)	11(3)					
1Imd	1.87(3)	3(4)	-4(1)	0.0556	120.652	13.714	11
0N/O							
1Imd	1.85(3)	10(3)					
1Imd	2.16(3)	18(3)					
1Imd	2.26(3)	12(4)					
1Imd	2.05(3)	19(3)					
1Imd	1.95(3)	17(3)	-3(1)	0.0715	154.924	17.609	11
3N/O	2.06(3)	8(3)					
1Imd	2.17(3)	2(2)	2(2)	0.1734	375.846	25.399	5
2N/O	2.06(3)	10(4)					
1Imd	2.02(2)	0(2)					
1Imd	2.17(2)	2(1)	0(1)	0.0831	180.250	14.084	7
1N/O	2.07(5)	6(6)					
1Imd	1.94(3)	2(3)					
1Imd	2.05(2)	6(2)					
1Imd	2.18(2)	5(2)	-2(2)	0.0732	158.669	14.694	9
0N/O							
1Imd	2.09(2)	12(3)					
1Imd	1.88(2)	5(4)					
1Imd	1.98(2)	11(3)					
1Imd	2.20(2)	10(2)	-3(2)	0.0945	204.907	18.977	9
2N/O	2.06(3)	5(3)					
1Imd	2.18(3)	1(2)	3(3)	0.2274	492.942	33.312	5
1N/O	2.06(5)	5(6)					
1Imd	2.17(2)	2(1)					
1Imd	2.02(2)	1(2)	0(2)	0.1316	285.249	22.289	7
0N/O							
1Imd	2.06(2)	8(2)					
1Imd	1.94(2)	4(3)					
1Imd	2.18(2)	7(2)	-2(2)	0.1353	293.394	22.925	7

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.03(7)	22(6)	-7(3)	0.0952	206.426	16.130	7
1S	2.28(2)	5(2)					
1Imd 0°	2.00(2)	4(2)					
3N/O	2.08(6)	21(10)	-2(2)	0.0631	136.739	12.664	9
1S	2.29(4)	13(7)					
1Imd 0°	2.00(2)	0(2)					
1Imd 0°	2.15(2)	1(2)					
3N/O	2.08(2)	8(2)	5(2)	5(2)	172.275	15.955	9
1S	2.74(7)	20(12)					
1Imd 0°	1.58(4)	16(5)					
1Imd 5°	2.20(2)	1(2)					
3N/O	2.04(6)	14(7)	-4(3)	0.0795	174.012	16.115	9
1S	2.29(5)	14(10)					
1Imd 0°	2.01(4)	6(4)					
1Imd 10°	2.15(3)	2(2)					
3N/O	2.05(6)	15(7)	-4(3)	0.0785	170.090	15.752	9
1S	2.29(5)	13(9)					
1Imd 5°	2.01(3)	5(3)					
1Imd 10°	2.15(3)	2(2)					
2N/O	2.08(6)	18(11)	-5(2)	0.0416	90.239	10.257	11
1S	2.31(3)	12(6)					
1Imd 0°	2.01(3)	4(2)					
1Imd 0°	2.14(3)	4(2)					
1Imd 0°	1.90(4)	2(4)					
2N/O	2.07(8)	20(13)	-4(2)	0.0467	101.334	11.518	11
1S	2.31(4)	13(7)					
1Imd 0°	1.94(5)	3(6)					
1Imd 0°	2.16(3)	3(2)					
1Imd 5°	2.03(4)	2(3)					
2N/O	2.00(5)	11(7)	-2(2)	0.047	101.817	11.573	11
1S	2.35(0.15)	33(33)					
1Imd 0°	2.01(3)	1(2)					
1Imd 0°	2.17(2)	1(2)					
1Imd 10°	2.13(3)	3(3)					
2N/O	2.09(9)	24(18)	-4(2)	0.0459	99.588	11.320	11
1S	2.30(3)	10(5)					
1Imd 0°	2.15(3)	3(2)					
1Imd 5°	1.92(5)	3(6)					
1Imd 5°	2.02(3)	3(3)					
2N/O	2.00(5)	11(6)	-2(2)	0.0445	96.586	10.978	11

1S	2.35(0.15)	33(33)					
1Imd 10°	2.01(3)	0(2)					
1Imd 5°	2.17(2)	1(2)					
1Imd 5°	2.12(4)	3(3)					
2N/O	1.94(3)	5(3)	-3(2)	0.039	84.593	9.615	11
1S	2.38(7)	21(14)					
1Imd 0°	2.13(4)	6(4)					
1Imd 10°	2.15(2)	5(1)					
1Imd 10°	2.02(2)	4(2)					
2N/O	1.94(3)	5(2)	-3(2)	0.0392	84.893	9.649	11
1S	2.38(7)	22(14)					
1Imd 5°	2.14(4)	5(4)					
1Imd 10°	2.15(2)	5(1)					
1Imd 10°	2.02(2)	4(2)					
2N/O	2.01(5)	11(7)	-2(2)	0.0454	98.399	11.184	11
1S	2.33(0.13)	31(28)					
1Imd 0°	2.16(3)	0(2)					
1Imd 5°	2.01(2)	0(2)					
1Imd 10°	2.14(3)	3(2)					

Co-N(2.0) Co-N(2.2) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(5)	9(9)	-2(2)	0.0454	98.491	11.195	11
1N/O	2.17(3)	0(3)					
1S	2.22(0.11)	23(25)					
1Imd 0°	2.15(3)	0(3)					
1Imd 0°	2.01(3)	0(2)					
1N/O			No Fit	No Fit	No Fit	No Fit	11
2N/O							
1S							
1Imd 0°							
1Imd 0°							
2N/O	1.96(3)	7(4)	-1(1)	0.0347	75.261	8.554	11
1N/O	2.16(2)	0(2)					
1S	1.85(9)	35(28)					
1Imd 0°	2.16(2)	1(2)					
1Imd 5°	2.02(2)	2(1)					
1N/O	1.95(4)	3(5)	-2(2)	0.039	84.536	9.609	11
2N/O	2.16(5)	3(3)					
1S	2.20(8)	14(14)					
1Imd 0°	2.15(2)	1(2)					
1Imd 5°	2.02(3)	1(2)					

2N/O	1.99(2)	6(3)	-3(2)	0.0304	65.943	7.495	11
1N/O	2.20(1)	2(1)					
1S	2.20(5)	18(10)					
1Imd 0°	2.08(3)	4(3)					
1Imd 10°	2.08(2)	1(2)					
1N/O	1.97(4)	2(3)	-2(2)	0.0405	87.704	9.969	11
2N/O	2.20(4)	0(2)					
1S	2.20(6)	5(6)					
1Imd 0°	2.09(4)	4(3)					
1Imd 10°	2.09(3)	2(3)					
2N/O	1.99(3)	6(3)	-3(2)	0.0317	68.823	7.823	11
1N/O	2.20(1)	2(1)					
1S	2.20(5)	18(11)					
1Imd 5°	2.09(3)	4(3)					
1Imd 10°	2.08(3)	1(2)					
1N/O	1.97(4)	2(3)	-2(2)	0.0417	90.515	10.288	11
2N/O	2.20(4)	0(2)					
1S	2.20(6)	5(6)					
1Imd 5°	2.09(4)	4(3)					
1Imd 10°	2.09(3)	2(3)					
1N/O			No Fit	No Fit	No Fit	No Fit	13
1N/O							
1S							
1Imd 0°							
1Imd 0°							
1Imd 5°							
1N/O	1.98(4)	2(4)	-4(2)	0.0305	66.103	9.724	13
1N/O	2.19(2)	2(2)					
1S	2.22(6)	15(10)					
1Imd 0°	2.09(5)	4(5)					
1Imd 0°	1.96(0.13)	12(17)					
1Imd 10°	2.08(3)	2(3)					
1N/O			No Fit	No Fit	No Fit	No Fit	13
1N/O							
1S							
1Imd 0°							
1Imd 5°							
1Imd 5°							
1N/O	1.98(4)	2(4)	-4(2)	0.0314	68.037	10.009	13
1N/O	2.19(2)	2(2)					
1S	2.22(6)	15(9)					
1Imd 10°	2.10(5)	3(5)					
1Imd 5°	1.97(0.14)	12(18)					

1Imd 5°	2.08(3)	2(3)					
1N/O	1.99(3)	2(4)	-5(2)	0.0266	57.620	8.476	13
1N/O	2.19(2)	3(1)					
1S	2.22(4)	15(9)					
1Imd 0°	2.07(3)	3(3)					
1Imd 10°	2.07(3)	1(2)					
1Imd 10°	1.91(5)	6(6)					
1N/O	1.99(4)	2(4)	-5(2)	0.028	60.666	8.924	13
1N/O	2.19(2)	3(1)					
1S	2.22(5)	15(9)					
1Imd 5°	2.08(3)	2(3)					
1Imd 10°	2.07(3)	0(2)					
1Imd 10°	1.91(5)	6(6)					
1N/O	1.98(4)	1(4)	-4(2)	0.0293	63.571	9.352	13
1N/O	2.19(2)	2(2)					
1S	2.23(6)	16(11)					
1Imd 0°	2.08(4)	3(4)					
1Imd 5°	1.92(8)	9(9)					
1Imd 10°	2.08(3)	1(2)					

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.03(7)	22(6)					
1S	2.29(2)	5(2)					
1Imd	2.00(2)	4(3)	-7(3)	0.0986	213.765	16.703	7
3N/O	2.08(5)	18(10)					
1S	2.29(6)	17(11)					
1Imd	2.16(2)	1(1)					
1Imd	2.01(2)	0(2)	-2(2)	0.0652	141.286	13.085	9
2N/O	2.08(6)	17(10)					
1S	2.31(4)	13(7)					
1Imd	2.01(3)	4(2)					
1Imd	2.14(3)	4(2)					
1Imd	1.90(4)	1(4)	-5(2)	0.0425	92.126	10.471	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.04(7)	22(6)					
1S	2.29(2)	5(2)					
1Imd	2.00(3)	4(3)	-7(4)	0.1014	219.784	17.173	7
3N/O	2.05(3)	14(5)					
1S	2.54(0.44)	54(80)	-1(2)	0.0646	140.027	12.968	9

1Imd	2.02(2)	0(2)					
1Imd	2.17(2)	2(1)					
2N/O	2.09(6)	16(10)					
1S	2.32(4)	14(8)					
1Imd	2.15(3)	4(2)					
1Imd	1.90(4)	1(4)					
1Imd	2.01(3)	4(2)	-5(2)	0.0432	93.764	10.658	11

Table E.3. Additional Fits for Zn(II) WT-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.17(2)	1(2)	14(4)	0.4648	9529.103	567.281	3
3N/O	2.16(2)	3(2)	11(0)	0.4315	8845.087	526.561	3
4N/O	2.14(3)	5(2)	9(3)	0.4366	8950.887	532.859	3
5N/O	2.13(3)	7(2)	7(3)	0.4621	9473.702	563.983	3
6N/O	2.12(3)	10(3)	5(4)	0.4956	10160.179	604.850	3
7N/O	2.10(4)	12(3)	3(4)	0.5307	10879.302	647.660	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.19(2)	4(1)	-1(4)	0.2439	4999.888	297.650	3
3S	2.27(2)	7(1)	-3(3)	0.2293	4700.192	279.809	3
4S	2.26(2)	9(1)	-6(3)	0.2488	5100.999	303.670	3
5S	2.26(2)	11(1)	-7(4)	0.2816	5772.987	343.674	3
6S	2.25(3)	13(2)	-9(4)	0.3183	6525.609	388.479	3
7S	2.24(3)	15(2)	-11(4)	0.3548	7273.150	432.981	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.08(2)	1(2)					
1N/O	2.21(2)	6(2)	8(3)	0.2987	6123.046	413.779	5
2N/O	2.04(3)	0(2)					
2N/O	2.18(2)	3(2)	5(3)	0.3329	6823.680	461.126	5
3N/O	2.08(3)	2(2)					
1N/O	2.20(2)	5(2)	6(3)	0.3120	6396.503	432.259	5
4N/O	2.07(3)	5(3)					
1N/O	2.19(2)	4(2)	4(3)	0.3428	7028.165	474.945	5
3N/O	2.04(3)	3(3)					
2N/O	2.18(2)	2(2)	3(3)	0.3630	7440.865	502.834	5

5N/O	2.06(3)	8(3)					
1N/O	2.18(2)	3(2)	2(3)	0.3802	7794.578	526.737	5
4N/O	2.03(3)	6(3)					
2N/O	2.17(2)	1(2)	2(3)	0.3990	8179.097	552.722	5
3N/O	2.00(4)	4(4)					
3N/O	2.16(2)	1(2)	1(3)	0.4216	8642.444	584.034	5
6N/O	2.05(4)	10(4)					
1N/O	2.18(2)	3(2)	1(4)	0.4183	8574.538	579.445	5
5N/O	2.03(4)	9(4)					
2N/O	2.16(3)	0(2)	0(4)	0.4344	8905.703	601.824	5
4N/O	2.00(4)	8(5)					
3N/O	2.15(3)	2(2)	0(4)	0.4549	9324.970	630.157	5

Zn-S(2.2) Zn-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.18(2)	4(2)					
1S	2.31(2)	1(1)	-9(3)	0.1466	3005.653	203.114	5
2S	2.14(3)	5(2)					
2S	2.28(2)	2(1)	-11(3)	0.1663	3409.251	230.388	5
3S	2.18(2)	8(2)					
1S	2.30(2)	0(1)	-11(3)	0.1600	3280.811	221.709	5
4S	2.27(2)	9(1)					
1S	1.07(0.15)	28(38)	-4(4)	0.2303	4720.229	318.981	5
3S	2.14(3)	9(3)					
2S	2.28(2)	3(1)	-13(4)	0.1888	3870.632	261.567	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.25(2)	6(1)					
2S	2.09(3)	7(3)	-14(4)	0.2206	4522.771	305.637	5
3S	2.11(3)	10(3)					
3S	2.26(2)	5(2)	-14(4)	0.2224	4558.549	308.055	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.27(3)	11(2)	-4(6)	0.2574	5276.609	356.579	5

2S	1.88(0.11)	35(25)					
4S	2.25(2)	6(2)					
3S	2.09(4)	10(4)	-15(4)	0.2440	5002.369	338.047	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	3(2)					5
1S	2.31(2)	0(1)	1(3)	0.1510	3095.498	209.186	
1N/O	1.99(3)	0(2)					5
2S	2.28(2)	3(1)	-3(3)	0.1623	3328.044	224.900	
2N/O	2.00(4)	6(3)					
2S	2.29(2)	4(1)	-3(4)	0.1806	3702.152	250.182	5
3N/O	2.06(4)	6(3)					
1S	2.31(2)	0(1)	1(4)	0.1646	3374.422	228.035	5
1N/O	2.14(0.23)	20(95)					
3S	2.28(3)	7(2)	-2(7)	0.2199	4508.682	304.685	5
1N/O	1.15(0.12)	7(10)					
4S	2.26(2)	9(1)	-7(3)	0.2671	5475.143	369.996	5
4N/O	2.07(5)	11(3)					
1S	2.30(2)	1(1)	1(4)	0.1850	3792.708	256.301	5
2N/O	2.20(0.18)	23(102)					
3S	2.29(3)	7(2)	0(12)	0.2104	4314.237	291.545	5
3N/O	2.17(0.11)	17(25)					
2S	2.30(2)	5(2)	4(9)	0.1886	3865.334	261.209	5
5N/O	2.08(8)	15(4)					
1S	2.30(2)	1(1)	1(6)	0.2047	4196.775	283.607	5
1N/O	2.45(2)	3(1)					
5S	2.23(3)	14(2)	-13(4)	0.1528	3132.486	211.685	5
4N/O	2.22(7)	21(22)					
2S	2.31(2)	4(1)	6(7)	0.1805	3700.700	250.084	5
2N/O	2.22(2)	2(1)					
4S	2.23(2)	6(1)	-6(4)	0.1494	3063.428	207.018	5
3N/O	2.23(0.10)	20(54)					
3S	2.29(2)	7(2)	2(11)	0.1991	4080.883	275.775	5

6N/O	2.10(0.11)	20(5)					
1S	2.30(2)	1(1)	2(7)	0.2217	4544.053	307.075	5
1N/O	2.44(2)	3(1)					
6S	2.22(4)	16(2)	-13(5)	0.1716	3517.553	237.707	5
5N/O	2.24(6)	25(16)					
2S	2.31(2)	4(1)	7(5)	0.1740	3567.483	241.081	5
2N/O	2.20(2)	1(1)					
5S	2.22(2)	8(1)	-8(4)	0.1629	3340.062	225.713	5
4N/O	2.26(5)	17(19)					
3S	2.30(2)	7(1)	6(5)	0.1852	3796.678	256.570	5
3N/O	2.23(2)	1(1)					
4S	2.24(2)	4(1)	-4(4)	0.1466	3005.416	203.098	5

Zn-N(2.0) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(3)	3(2)					5
1Br	2.43(2)	4(1)	1(5)	0.1705	3495.642	236.226	
1N/O	1.42(9)	11(12)					5
2Br	2.36(3)	7(1)	-18(8)	0.2883	5910.990	399.449	
2N/O	2.00(4)	5(2)					
2Br	2.39(2)	7(1)	-10(6)	0.1461	2995.317	202.416	5
3N/O	2.08(3)	5(2)					
1Br	2.43(2)	4(1)	1(4)	0.1393	2855.550	192.971	5
1N/O	1.41(9)	11(11)					
3Br	2.35(3)	9(1)	-20(7)	0.2372	4863.143	328.638	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.02(2)	0(2)					
1Br	2.10(2)	2(1)	0(3)	0.2305	4725.830	319.359	5
2N/O	1.96(4)	6(3)					
3Br	2.37(2)	9(1)	-16(5)	0.1294	2652.328	179.237	5
3N/O	2.03(4)	7(2)					
2Br	2.41(2)	7(1)	-6(5)	0.1240	2541.453	171.745	5
5N/O	2.02(3)	3(2)					
1Br	2.10(2)	3(2)	-1(4)	0.2849	5840.780	394.705	5

1N/O 5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 2Br	2.04(4) 2.41(2)	10(2) 7(1)	-5(4)	0.1147	2351.770	158.926	5
2N/O 4Br	1.93(4) 2.36(2)	6(3) 10(1)	-19(5)	0.1241	2543.715	171.898	5
3N/O 3Br	1.97(4) 2.38(2)	9(3) 9(1)	-13(5)	0.1178	2414.911	163.193	5
6N/O 1Br	2.03(4) 2.09(3)	7(3) 5(2)	-2(4)	0.3313	6791.917	458.980	5
1N/O 6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O 2Br	2.03(4) 2.41(2)	12(2) 7(1)	-6(4)	0.1139	2335.564	157.831	5
2N/O 5Br	1.92(4) 2.35(2)	7(3) 12(1)	-20(5)	0.1254	2570.259	173.691	5
4N/O 3Br	1.99(4) 2.39(2)	12(3) 9(1)	-11(5)	0.1126	2308.905	156.030	5
3N/O 4Br	1.94(4) 2.37(2)	10(3) 11(1)	-17(5)	0.1176	2410.275	162.880	5

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O 1S 1Br	1.99(6) 2.24(7) 2.41(2)	7(4) 3(2) 5(2)	-8(8)	0.0843	1728.802	135.085	7
1N/O 2S 1Br	1.95(0.10) 2.21(9) 2.40(3)	6(9) 7(3) 5(2)	-12(10)	0.0869	1781.224	139.181	7
1N/O 1S 2Br	1.98(5) 2.26(6) 2.41(3)	1(3) 3(4) 9(3)	-7(7)	0.0955	1957.554	152.960	7
3N/O 1S 1Br	2.01(7) 2.24(6) 2.41(2)	11(4) 4(3) 5(2)	-7(8)	0.0837	1716.114	134.094	7

2N/O	2.00(9)	12(11)					
2S	2.23(9)	9(4)					
1Br	2.40(2)	5(2)	-9(10)	0.0852	1747.584	136.553	7
2N/O	2.00(5)	6(3)					
1S	2.29(4)	4(4)					
2Br	2.41(2)	10(3)	-5(5)	0.0841	1724.478	134.747	7

Zn-N(2.0) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(4)	11(4)					
1Imd	2.19(3)	0(3)	3(4)	0.3928	8053.411	544.228	5
4N/O	2.04(6)	15(8)					
1Imd	2.09(3)	4(3)					
1Imd	2.22(3)	5(2)	1(3)	0.3108	6371.215	497.835	7
3N/O	2.05(0.10)	20(16)					
1Imd	2.09(3)	11(2)					
1Imd	2.22(2)	11(2)					
1Imd	1.98(3)	7(3)	-2(3)	0.2284	4683.058	433.703	9
2N/O	2.12(3)	1(4)					
1Imd	1.88(2)	11(3)					
1Imd	1.98(2)	17(2)					
1Imd	2.21(2)	15(2)					
1Imd	2.09(2)	18(2)	-4(2)	0.1639	3360.880	382.011	11
1N/O	2.13(4)	3(3)					
1Imd	2.21(3)	16(3)					
1Imd	1.88(4)	12(5)					
1Imd	1.96(3)	18(4)					
1Imd	2.10(3)	19(3)					
1Imd	1.73(0.22)	16(33)	-4(4)	0.1328	2722.955	400.561	13
4N/O	2.09(4)	9(4)					
1Imd	2.20(3)	1(3)	4(4)	0.3746	7678.663	518.904	5
3N/O	2.05(6)	12(8)					
1Imd	2.22(3)	5(2)					
1Imd	2.09(3)	5(3)	1(3)	0.3018	6187.927	483.513	7
2N/O	2.11(5)	4(6)					
1Imd	2.21(2)	10(2)					
1Imd	2.08(2)	11(2)					
1Imd	1.96(3)	8(3)	-1(3)	0.2126	4358.762	403.669	9
1N/O	2.13(3)	3(3)					
1Imd	2.10(2)	18(2)	-4(2)	0.1435	2941.292	334.319	11

1Imd	1.99(2)	17(2)					
1Imd	1.89(2)	11(3)					
1Imd	2.22(2)	15(2)					
0N/O							
1Imd	2.05(4)	23(7)					
1Imd	2.25(3)	18(7)					
1Imd	2.15(4)	22(7)					
1Imd	1.86(5)	12(6)					
1Imd	1.95(5)	20(7)	-5(3)	0.2076	4255.040	483.645	11
3N/O	2.09(4)	6(4)					
1Imd	2.21(3)	1(3)	5(4)	0.3700	7585.867	512.633	5
2N/O	2.05(7)	9(9)					
1Imd	2.10(3)	5(3)					
1Imd	2.22(3)	6(2)	2(3)	0.3048	6247.894	488.199	7
1N/O	2.13(4)	1(4)					
1Imd	1.97(2)	8(2)					
1Imd	2.21(2)	11(2)					
1Imd	2.09(2)	12(2)	-1(3)	0.2000	4100.904	379.789	9
0N/O							
1Imd	1.90(3)	10(3)					
1Imd	2.11(2)	18(2)					
1Imd	2.00(2)	16(3)					
1Imd	2.23(2)	15(2)	-4(2)	0.1996	4091.649	378.932	9
2N/O	2.10(5)	4(5)					
1Imd	2.21(4)	1(3)	7(4)	0.3926	8048.316	543.884	5
1N/O	2.04(0.10)	6(13)					
1Imd	2.09(3)	5(3)					
1Imd	2.22(3)	6(2)	3(4)	0.3307	6779.684	529.752	7
0N/O							
1Imd	2.10(2)	12(2)					
1Imd	2.22(2)	11(1)					
1Imd	1.98(3)	8(2)	-1(3)	0.2400	4919.432	384.395	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.99(4)	7(4)					
1S	2.30(1)	1(1)					
1Imd	2.06(2)	1(2)	-1(3)	0.0879	1811.714	141.564	7
1N/O	2.00(2)	2(2)					
1S	2.29(1)	2(1)					
1Imd	2.05(2)	3(1)	-5(2)	0.0616	1262.334	116.906	9

1Imd	1.89(3)	0(3)					
0N/O							
1S	2.29(1)	0(1)					
1Imd	1.92(3)	4(3)					
1Imd	2.16(4)	4(4)					
1Imd	2.04(2)	7(3)	-2(2)	0.0641	1314.055	121.696	11

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	8(4)					
1S	2.30(1)	0(1)					
1Imd	2.06(2)	1(2)	-2(3)	0.0862	1766.225	138.009	7
1N/O	1.98(3)	2(4)					
1S	2.31(1)	1(1)					
1Imd	2.21(0.19)	22(73)					
1Imd	2.07(2)	1(2)	0(4)	0.0708	1452.377	134.506	9
0N/O							
1S	2.29(1)	0(1)					
1Imd	1.92(3)	4(3)					
1Imd	2.04(2)	7(2)					
1Imd	2.16(4)	4(4)	-2(2)	0.0599	1226.983	113.632	11

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	8(4)					
1S	2.30(1)	0(1)					
1Imd	2.06(2)	0(2)	-2(3)	0.0853	1748.956	136.660	7
1N/O	2.00(2)	1(3)					
1S	2.29(1)	2(1)					
1Imd	1.89(3)	0(3)					
1Imd	2.05(2)	3(1)	-5(2)	0.0595	1219.561	112.945	9
0N/O							
1S	2.29(1)	0(1)					
1Imd	2.17(3)	4(4)					
1Imd	2.04(2)	7(2)					
1Imd	1.92(3)	4(2)	-2(2)	0.0575	1178.060	109.101	11

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(3)	2(2)					
1S	2.66(3)	0(2)					
1Imd	2.00(3)	2(2)	-1(4)	0.3018	6187.946	483.514	7

1N/O	2.15(2)	5(2)					
1S	2.66(2)	0(2)					
1Imd	2.09(5)	2(8)					
1Imd	1.99(4)	3(4)	-2(3)	0.1987	4073.736	377.273	9
0N/O							
1S	2.67(3)	3(3)					
1Imd	2.18(2)	11(2)					
1Imd	2.06(2)	12(2)					
1Imd	1.94(2)	8(2)	-1(3)	0.2081	4265.693	395.050	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	3(2)					
1S	2.29(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0236	483.534	44.781	9
0N/O							
1S	2.29(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)	-5(1)	0.016	328.726	30.444	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	3(2)					
1S	2.29(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0226	464.225	42.992	9
0N/O							
1S	2.29(2)	4(2)					
1Br	2.41(1)	5(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)	-5(1)	0.0163	333.354	30.872	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(2)					
1S	2.29(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0219	449.377	41.617	9
0N/O			-5(1)	0.0165	338.610	31.359	9

1S	2.29(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.07(2)	1(1)					
1Imd	1.95(2)	0(2)					

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)					
1S	2.29(2)	2(1)					
1Br	2.41(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0249	511.335	47.355	9
0N/O							
1S	2.29(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	1.95(2)	0(2)					
1Imd	2.07(2)	2(1)	-5(1)	0.0155	318.046	29.455	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)					
1S	2.29(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0239	490.843	45.457	9
0N/O							
1S	2.29(2)	4(2)					
1Br	2.41(1)	5(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)	-5(1)	0.0156	320.159	29.650	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	3(2)					
1S	2.29(2)	2(1)					
1Br	2.42()	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0232	474.897	43.981	9
0N/O							
1S	2.29(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)	-5(1)	0.0158	323.372	29.948	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)					
1S	2.29(2)	3(2)					
1Br	2.41(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0262	536.784	49.712	9
0N/O							
1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)	-5(1)	0.0153	314.445	29.121	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)					
1S	2.29(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0251	515.464	47.738	9
0N/O							
1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)	-5(1)	0.0154	314.941	29.167	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)					
1S	2.29(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0243	498.800	46.194	9
0N/O							
1S	2.30(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)	-5(1)	0.0155	316.862	29.345	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
1S	2.29(2)	3(2)					
1Br	2.41(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0273	562.084	52.055	9
0N/O			-5(1)	0.0152	312.059	28.900	9

1S	2.30(2)	5(2)					
1Br	2.40(1)	5(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.95(2)	0(2)					

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)					
1S	2.29(2)	2(2)					
1Br	2.41(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0262	536.977	49.730	9
0N/O							
1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	1.95(2)	0(2)					
1Imd	2.07(2)	2(1)	-5(1)	0.0152	311.015	28.803	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)					
1S	2.29(2)	2(2)					
1Br	2.41(1)	7(2)					
1Imd	2.05(2)	0(1)	-4(2)	0.0262	536.977	49.730	9
0N/O							
1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	1.95(2)	0(2)					
1Imd	2.07(2)	2(1)	-5(1)	0.0152	311.015	28.803	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(2)	-4(2)	0.0253	519.615	48.122	9
1S	2.29(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd 0°	2.05(2)	0(1)					
0N/O			-5(1)	0.0152	311.725	28.869	9
1S	2.30(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd 0°	2.07(2)	2(1)					
1Imd 0°	1.95(2)	0(2)					

0N/O			-5(2)	0.0177	363.442	33.659	9
1S	2.30(2)	3(2)					
1Br	2.41(1)	6(1)					
1Imd 0°	2.06(2)	2(1)					
1Imd 5°	1.94(2)	0(2)					
0N/O			-5(2)	0.0256	525.671	48.683	9
1S	2.28(2)	2(1)					
1Br	2.42(1)	7(2)					
1Imd 0°	2.04(2)	1(1)					
1Imd 10°	1.96(3)	5(3)					
0N/O			-6(3)	0.0327	670.424	62.089	9
1S	2.27(3)	2(1)					
1Br	2.42(1)	6(2)					
1Imd 5°	2.04(2)	0(2)					
1Imd 10°	1.94(3)	3(3)					

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.01(6)	15(7)					
1S	2.30(1)	0(1)					
1Imd	2.05(2)	0(2)	-2(3)	0.1034	2118.990	165.574	7
2N/O	2.47(1)	1(1)					
1S	2.29(2)	3(2)					
1Imd	1.94(2)	1(2)					
1Imd	2.07(2)	3(1)	-6(2)	0.0265	544.224	50.401	9
1N/O	1.99(3)	0(4)					
1S	2.28(1)	1(1)					
1Imd	2.47(3)	2(4)					
1Imd	2.04(2)	3(1)					
1Imd	1.88(3)	1(3)	-7(2)	0.0413	846.293	96.193	11

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.02(7)	17(7)					
1S	2.30(1)	0(1)					
1Imd	2.05(2)	0(2)	-2(3)	0.1002	2054.341	160.522	7
2N/O	2.47(1)	1(1)					
1S	2.29(2)	3(2)					
1Imd	1.94(2)	1(2)					
1Imd	2.06(2)	3(1)	-6(2)	0.0282	578.383	53.565	9
1N/O	1.99(3)	1(4)					
1S	2.28(1)	1(1)	-7(2)	0.0406	831.384	94.499	11

1Imd	2.04(2)	3(1)					
1Imd	1.88(3)	1(3)					
1Imd	2.47(3)	2(4)					

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.03(8)	18(8)					
1S	2.30(1)	0(1)					
1Imd	2.05(2)	0(2)	-1(3)	0.0981	2011.131	157.146	7
2N/O	2.47(1)	1(1)					
1S	2.29(2)	3(2)					
1Imd	2.06(2)	3(1)					
1Imd	1.94(2)	1(2)	-6(2)	0.0297	609.494	56.446	9
1N/O	1.99(3)	1(4)					
1S	2.28(1)	1(1)					
1Imd	2.47(3)	2(4)					
1Imd	1.88(3)	1(3)					
1Imd	2.04(2)	2(1)	-7(2)	0.0409	838.498	95.307	11

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(4)	7(5)					
1S	2.68(4)	3(3)					
1Imd	2.16(4)	0(3)	4(4)	0.3196	6552.508	512.001	7
2N/O	2.01(4)	1(4)					
1S	3.14(3)	1(3)					
1Imd	2.09(3)	8(2)					
1Imd	2.21(2)	8(2)	4(3)	0.2505	5135.548	475.608	9
1N/O	1.98(0.15)	11(27)					
1S	2.67(3)	3(3)					
1Imd	1.95(4)	7(3)					
1Imd	2.19(3)	10(2)					
1Imd	2.06(3)	11(3)	-1(3)	0.1806	3702.216	420.809	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	11(4)					
1S	2.29(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0284	583.010	53.993	9
1N/O	1.95(4)	11(7)	-4(1)	0.0116	237.133	26.953	11

1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	1.97(2)	1(3)					
1Imd	2.08(2)	1(2)					
0N/O							
1S	2.29(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	2.05(0.21)	0(6)					
1Imd	2.09(0.32)	4(38)					
1Imd	1.93(9)	2(10)	-4(2)	0.0122	249.679	28.380	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.98(4)	10(4)	-4(2)	0.0277	568.128	52.615	9
1S	2.29(2)	3(2)					
1Br	2.41(1)	6(1)					
1Imd 0°	2.05(2)	1(1)					
1N/O	1.94(4)	10(6)	-4(1)	0.0114	234.559	26.661	11
1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd 0°	1.97(2)	1(3)					
1Imd 0°	2.08(2)	1(2)					
1N/O	1.94(3)	7(4)	-4(1)	0.0117	240.469	27.333	11
1S	2.30(2)	7(3)					
1Br	2.41(1)	5(1)					
1Imd 0°	1.99(2)	0(3)					
1Imd 5°	2.10(2)	1(2)					
1N/O	1.93(2)	1(1)	-3(1)	0.0102	208.695	23.721	11
1S	2.29(2)	6(3)					
1Br	2.42(1)	5(1)					
1Imd 0°	2.05(1)	0(1)					
1Imd 10°	2.11(3)	3(2)					
1N/O	1.94(2)	1(1)	-3(1)	0.0139	285.062	32.401	11
1S	2.29(2)	7(3)					
1Br	2.42(1)	5(1)					
1Imd 5°	2.06(1)	0(1)					
1Imd 10°	2.12(3)	2(3)					
0N/O			-5(2)	0.0126	257.385	29.255	11
1S	2.29(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	2.08(4)	0(4)					
1Imd	1.97(9)	3(9)					
1Imd	1.99(0.26)	12(23)					

0N/O			-19(4)	0.0451	925.059	105.146	11
1S	2.18(3)	3(3)					
1Br	2.39(2)	3(1)					
1Imd 0°	2.33(4)	1(4)					
1Imd 5°	1.05(6)	7(6)					
1Imd 10°	1.90(5)	5(4)					

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	10(4)					
1S	2.29(2)	3(2)					
1Br	2.42(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0272	557.728	51.652	9
1N/O	1.94(4)	10(6)					
1S	2.30(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	1.98(2)	1(3)					
1Imd	2.08(2)	1(2)	-4(1)	0.0114	234.386	26.641	11
0N/O							
1S	2.29(2)	5(2)					
1Br	2.41(1)	6(1)					
1Imd	1.98(0.26)	12(24)					
1Imd	2.08(5)	0(4)					
1Imd	1.97(9)	3(9)	-5(2)	0.013	265.582	30.187	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	11(4)					
1S	2.30(3)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.029	595.210	55.123	9
1N/O	1.95(5)	12(7)					
1S	2.30(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.97(2)	1(3)	-4(1)	0.0114	234.702	26.677	11
0N/O							
1S	2.30(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	2.05(0.11)	0(8)					
1Imd	2.11(0.16)	3(21)					
1Imd	1.93(4)	1(6)	-4(1)	0.0114	232.911	26.474	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	11(4)					
1S	2.30(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0283	579.715	53.688	9
1N/O	1.95(4)	11(7)					
1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	1.97(2)	1(3)					
1Imd	2.08(2)	1(2)	-4(1)	0.0113	231.682	26.334	11
0N/O							
1S	2.30(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	1.93(6)	2(8)					
1Imd	2.05(0.18)	0(8)					
1Imd	2.10(0.24)	4(30)	-4(2)	0.0117	238.844	27.148	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	11(4)					
1S	2.29(2)	3(2)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0277	568.667	52.665	9
1N/O	1.94(4)	11(6)					
1S	2.30(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.97(2)	1(3)	-4(1)	0.0113	231.031	26.260	11
0N/O							
1S	2.30(2)	5(2)					
1Br	2.41(1)	6(1)					
1Imd	2.10(0.25)	4(31)					
1Imd	1.93(6)	2(9)					
1Imd	2.05(0.18)	0(9)	-4(2)	0.012	245.362	27.889	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	11(5)					
1S	2.30(3)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0297	608.056	56.313	9

1N/O	1.96(5)	13(8)					
1S	2.31(2)	6(3)					
1Br	2.41(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.97(2)	1(2)	-4(1)	0.0115	236.416	26.872	11
0N/O							
1S	2.30(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	2.04(7)	1(7)					
1Imd	1.93(3)	1(5)					
1Imd	2.12(0.11)	2(15)	-4(1)	0.0109	224.237	25.488	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	11(4)					
1S	2.30(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0289	592.342	54.857	9
1N/O	1.95(5)	12(7)					
1S	2.31(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	1.97(2)	1(3)					
1Imd	2.08(2)	1(2)	-4(1)	0.0114	233.364	26.525	11
0N/O							
1S	2.30(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	1.93(4)	1(6)					
1Imd	2.04(0.10)	0(8)					
1Imd	2.11(0.14)	3(20)	-4(1)	0.0112	228.983	26.027	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	11(4)					
1S	2.30(2)	4(2)					
1Br	2.41(1)	6(2)					
1Imd	2.05(2)	1(1)	-4(2)	0.0283	581.022	53.809	9
1N/O	1.95(4)	11(7)					
1S	2.31(2)	5(2)					
1Br	2.41(1)	5(1)					
1Imd	1.97(2)	1(3)					
1Imd	2.08(2)	1(2)	-4(1)	0.0113	232.584	26.437	11
0N/O							
1S	2.30(2)	5(2)	-4(1)	0.0114	234.311	26.633	11

1Br	2.41(1)	6(1)					
1Imd	1.93(4)	2(6)					
1Imd	2.11(0.14)	3(19)					
1Imd	2.04(0.10)	0(8)					

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	12(5)					
1S	2.30(3	4(3)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(3)	0.0301	617.238	57.163	9
1N/O	1.97(6)	14(9)					
1S	2.31(2)	6(3)					
1Br	2.40(1)	5(1)					
1Imd	1.96(2)	1(2)					
1Imd	2.08(2)	1(2)	-5(1)	0.0116	237.067	26.946	11
0N/O							
1S	2.30(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	1.93(3)	1(5)					
1Imd	2.12(8)	2(13)					
1Imd	2.04(5)	1(6)	-4(1)	0.0106	217.176	24.685	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	12(5)					
1S	2.30(3)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0293	601.054	55.664	9
1N/O	1.96(5)	13(8)					
1S	2.31(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.97(2)	1(2)	-5(1)	0.0114	233.952	26.592	11
0N/O							
1S	2.30(2)	6(2)					
1Br	2.41(1)	5(1)					
1Imd	2.04(7)	1(7)					
1Imd	1.93(3)	1(5)					
1Imd	2.12(0.10)	2(15)	-4(1)	0.0108	220.739	25.090	11

APPENDIX F

ADDITIONAL FIT TABLES FOR GLUTAMATE 34 MUTATIONS

Table F.1. Additional Fits for Ni(II) E34A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

	Ni-N(2.0)						
N	**Radius Å**	**σ^2 (x10^{-3} $Å^2$)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(4)	2(2)	5(11)	0.4311	2559.525	376.574	3
3N/O	2.08(3)	1(2)	6(7)	0.3278	1946.268	286.347	3
4N/O	2.08(3)	1(2)	5(5)	0.2628	1560.172	229.543	3
5N/O	2.08(2)	2(2)	5(4)	0.2248	1334.606	196.356	3
6N/O	2.09(2)	3(2)	5(4)	0.2069	1228.575	180.756	3
7N/O	2.09(2)	4(2)	5(4)	0.2044	1213.420	178.526	3

	Ni-S(2.2)						
N	**Radius Å**	**σ^2 (x10^{-3} $Å^2$)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.17(4)	2(2)	neg17(12)	0.3626	2152.503	316.690	3
3S	2.17(4)	4(2)	neg16(9)	0.2885	1712.826	252.002	3
4S	2.18(3)	5(2)	neg16(7)	0.2525	1499.320	220.590	3
5S	2.18(3)	7(2)	neg16(7)	0.2390	1419.069	208.782	3
6S	2.18(3)	8(2)	neg16(7)	0.2393	1420.761	209.031	3
7S	2.18(3)	9(2)	neg17(6)	0.2481	1473.089	216.730	3

	Ni-N(2.0) Ni-N(2.2)						
	r(Å)	**σ^2(x10^{-3} $Å^2$)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.05(2)	7(2)					
1N/O	2.18(3)	10(2)	7(5)	0.1799	1068.266	222.700	5
2N/O	2.03(2)	7(2)					
2N/O	2.16(2)	7(2)	6(4)	0.1517	900.741	187.777	5
3N/O	2.13(2)	5(2)					
1N/O	2.00(2)	9(2)	7(4)	0.1570	932.319	194.360	5
4N/O	2.13(2)	3(2)					
1N/O	2.00(2)	8(2)	6(4)	0.1474	875.352	182.484	5
3N/O	2.04(2)	4(2)					
2N/O	2.18(3)	6(2)	6(4)	0.1485	881.831	183.834	5
5N/O	2.12(2)	1(2)					
1N/O	1.99(3)	7(2)	6(4)	0.1545	917.518	191.274	5

4N/O	2.05(2)	2(2)					
2N/O	2.18(3)	5(3)	5(4)	0.1615	959.126	199.948	5
3N/O	2.03(3)	3(2)					
3N/O	2.16(3)	3(3)	5(4)	0.1660	985.825	205.514	5
6N/O	2.07(3)	1(2)					
1N/O	2.21(4)	6(3)	5(4)	0.1769	1050.292	218.953	5
5N/O	2.05(3)	1(2)					
2N/O	2.19(4)	3(4)	5(4)	0.1847	1096.620	228.611	5
4N/O	2.04(3)	1(3)					
3N/O	2.17(4)	2(4)	5(4)	0.1898	1127.039	234.953	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.14(4)	2(2)					
1S	2.28(4)	5(2)	neg14(8)	0.1959	1163.242	242.500	5
2S	2.13(4)	1(2)					
2S	2.26(4)	1(3)	neg14(8)	0.2012	1194.338	248.982	5
3S	2.15(4)	1(2)					
1S	2.29(5)	3(3)	neg14(8)	0.1990	1181.726	246.353	5
4S	2.16(4)	3(2)					
1S	2.30(6)	2(4)	neg15(8)	0.2137	1268.695	264.484	5
3S	2.14(4)	1(3)					
2S	2.27(5)	1(4)	neg14(8)	0.2158	1281.466	267.146	5
5S	2.19(5)	7(4)					
1S	2.37(0.4)	16(104)	neg14(12)	0.2338	1388.237	289.404	5
4S	2.15(5)	4(4)					
2S	2.28(9)	3(7)	neg15(9)	0.2326	1380.720	287.837	5
3S	2.14(6)	3(5)					
3S	2.26(9)	5(8)	neg15(9)	0.2325	1380.545	287.801	5
6S	2.17(5)	7(3)					
1S	1.92(0.17)	11(19)	neg18(12)	0.2317	1375.483	286.746	5
5S	2.19(4)	7(3)					
2S	2.39(0.20)	17(46)	neg13(10)	0.2278	1352.497	281.954	5
4S	2.19(4)	6(3)	neg12(13)	0.2307	1369.740	285.548	5

3S	2.32(0.25)	19(46)

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(3)	4(2)					5
1S	2.27(4)	3(2)	neg2(8)	0.1937	1150.064	239.753	
1N/O	1.99(4)	6(2)					5
2S	2.24(4)	1(2)	neg7(8)	0.2078	1233.967	257.244	
2N/O	2.01(4)	2(2)					
2S	2.26(4)	2(3)	neg5(8)	0.2026	1202.757	250.738	5
3N/O	2.03(3)	2(2)					
1S	2.28(4)	2(3)	neg1(7)	0.1824	1082.859	225.743	5
1N/O	1.99(4)	4(3)					
3S	2.23(4)	4(3)	neg8(8)	0.2074	1231.122	256.651	5
1N/O	1.83(0.55)	16(102)					
4S	2.18(5)	5(2)	neg17(12)	0.2487	1476.716	307.850	5
4N/O	2.04(3)	1(2)					
1S	2.29(4)	1(3)	neg1(6)	0.1852	1099.720	229.258	5
2N/O	2.01(5)	1(3)					
3S	2.24(6)	5(4)	neg7(9)	0.2139	1269.732	264.700	5
3N/O	2.02(5)	1(3)					
2S	2.26(5)	3(4)	neg3(8)	0.2063	1224.915	255.357	5
5N/O	2.05(4)	2(2)					
1S	2.29(6)	1(5)	1(6)	0.1953	1159.732	241.768	5
1N/O	1.73(7)	2(7)					
5S	2.17(4)	7(2)	neg18(8)	0.2226	1321.764	275.547	5
4N/O	2.04(5)	2(3)					
2S	2.26(7)	5(6)	neg2(8)	0.2118	1257.630	262.177	5
2N/O	2.02(6)	1(5)					
4S	2.23(7)	8(4)	neg8(10)	0.2213	1313.665	273.859	5
3N/O	2.03(6)	1(4)					
3S	2.24(7)	7(5)	neg5(9)	0.2193	1301.883	271.402	5
6N/O	2.07(5)	4(3)					
1S	2.27(9)	5(12)	1(7)	0.2044	1213.374	252.951	5

1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.06(6)	4(4)					
2S	2.25(8)	8(11)	neg1(9)	0.2146	1274.071	265.604	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.05(5)	3(5)					
3S	2.24(8)	9(8)	neg4(10)	0.2219	1317.384	274.634	5
3N/O	2.04(5)	2(5)					
4S	2.23(8)	10(7)	neg7(10)	0.2252	1337.170	278.758	5

Table F.2. Additional Fits for Ni(II) E34A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(3)	2(2)	5(7)	0.4513	2851.443	169.750	3
3N/O	2.08(2)	1(1)	5(5)	0.3553	2244.885	133.641	3
4N/O	2.08(2)	1(1)	5(4)	0.2954	1866.866	111.137	3
5N/O	2.08(2)	2(1)	5(3)	0.2611	1649.957	98.224	3
6N/O	2.08(2)	3(1)	5(3)	0.2457	1552.706	92.435	3
7N/O	2.08(2)	4(1)	4(3)	0.2447	1546.011	92.036	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(3)	2(1)	-17(8)	0.3879	2451.365	145.933	3
3S	2.17(2)	4(1)	-17(6)	0.3195	2018.660	120.174	3
4S	2.18(2)	5(1)	-16(5)	0.2866	1811.041	107.814	3
5S	2.18(2)	7(1)	-16(5)	0.2747	1735.834	103.337	3
6S	2.18(2)	8(1)	-16(5)	0.2757	1741.840	103.694	3
7S	2.18(2)	9(1)	-17(5)	0.2845	1797.853	107.029	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.05(2)	6(1)					
1N/O	2.18(2)	8(2)	7(4)	0.2605	1645.785	111.218	5
2N/O	2.03(2)	6(1)					
2N/O	2.16(2)	6(2)	6(3)	0.2249	1420.834	96.016	5
3N/O	2.13(2)	5(2)					
1N/O	2.00(2)	8(2)	6(3)	0.2272	1435.437	97.003	5

4N/O	2.12(2)	2(2)					
1N/O	2.00(2)	7(2)	6(3)	0.2129	1344.992	90.891	5
3N/O	2.04(2)	3(1)					
2N/O	2.17(2)	5(2)	6(3)	0.2140	1352.364	91.389	5
5N/O	2.12(2)	1(2)					
1N/O	2.00(2)	6(2)	6(3)	0.2146	1356.183	91.647	5
4N/O	2.05(2)	2(2)					
2N/O	2.18(2)	3(2)	5(3)	0.2199	1389.823	93.921	5
3N/O	2.03(2)	2(2)					
3N/O	2.16(2)	2(2)	5(3)	0.2226	1406.409	95.041	5
6N/O	2.07(2)	1(1)					
1N/O	2.21(3)	4(3)	5(3)	0.2314	1462.305	98.819	5
5N/O	2.06(2)	1(2)					
2N/O	2.19(3)	2(3)	5(3)	0.2363	1493.126	100.902	5
4N/O	2.04(2)	1(2)					
3N/O	2.17(3)	1(4)	5(3)	0.2392	1511.627	102.152	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.15(3)	2(1)					
1S	2.28(3)	4(2)	-14(6)	0.2522	1593.697	107.698	5
2S	2.13(3)	1(2)					
2S	2.26(3)	1(2)	-14(5)	0.2480	1566.970	105.892	5
3S	2.16(3)	1(1)					
1S	2.29(3)	3(2)	-14(5)	0.2465	1557.634	105.261	5
4S	2.17(3)	3(1)					
1S	2.30(4)	1(3)	-14(5)	0.2547	1609.205	108.746	5
3S	2.15(3)	2(2)					
2S	2.28(4)	1(3)	-14(5)	0.2561	1618.369	109.365	5
5S	2.21(2)	6(1)					
1S	2.42(6)	19(11)	-8(5)	0.2458	1553.311	104.969	5
4S	2.16(3)	4(3)					
2S	2.29(6)	4(5)	-14(6)	0.2684	1695.771	114.596	5
3S	2.15(4)	4(3)	-14(6)	0.2681	1693.776	114.461	5

3S	2.26(6)	6(6)					
6S	2.17(3)	7(2)					
1S	1.92(0.10)	10(11)	-19(7)	0.2670	1687.371	114.028	5
5S	2.19(3)	7(2)					
2S	2.38(0.13)	17(30)	-13(7)	0.2647	1672.576	113.028	5
4S	2.18(2)	5(2)					
3S	2.32(0.15)	19(28)	-13(8)	0.2667	1685.029	113.870	5

Ni-N(2.0) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.03(2)	4(1)					5
1S	2.27(3)	2(2)	-1(5)	0.2558	1616.264	109.223	
1N/O	1.99(3)	5(2)					5
2S	2.24(3)	1(2)	-7(6)	0.2663	1683.022	113.734	
2N/O	2.01(3)	2(2)					
2S	2.25(3)	2(2)	-5(5)	0.2524	1594.817	107.774	5
3N/O	2.04(2)	2(1)					
1S	2.28(3)	1(2)	-1(5)	0.2366	1495.161	101.039	5
1N/O	1.99(3)	4(2)					
3S	2.23(3)	4(2)	-9(6)	0.2565	1621.017	109.544	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.05(2)	1(1)					
1S	2.29(3)	1(3)	1(4)	0.2335	1475.180	99.689	5
2N/O	2.02(3)	1(2)					
3S	2.24(4)	6(3)	-7(6)	0.2565	1620.894	109.536	5
3N/O	2.03(3)	1(2)					
2S	2.26(4)	4(3)	-3(5)	0.2500	1579.905	106.766	5
5N/O	2.05(3)	2(2)					
1S	2.29(4)	2(4)	1(4)	0.2388	1509.005	101.975	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.04(3)	2(2)					
2S	2.26(5)	6(4)	-2(5)	0.2518	1591.069	107.520	5

2N/O	2.02(3)	1(3)					
4S	2.23(5)	8(3)	-8(6)	0.2601	1643.781	111.082	5
3N/O	2.03(3)	1(2)					
3S	2.24(5)	7(4)	-5(6)	0.2585	1633.490	110.387	5
6N/O	2.07(3)	4(2)					
1S	2.26(7)	6(10)	2(4)	0.2442	1542.976	104.270	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.06(3)	3(2)					
2S	2.25(6)	9(7)	-1(5)	0.2530	1598.676	108.034	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.05(3)	3(3)					
3S	2.24(5)	10(6)	-4(6)	0.2597	1641.009	110.895	5
3N/O	2.04(3)	2(3)					
4S	2.23(5)	10(4)	-7(7)	0.2626	1659.611	112.152	5

Ni-N(2.0) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.09(2)	2(2)					
1Imd	2.00(0.13)	6(16)	4(3)	0.2492	1574.932	106.430	5
4N/O	2.09(3)	1(3)					
1Imd	2.02(7)	1(5)					
1Imd	2.19(7)	1(6)	6(3)	0.2596	1640.476	128.184	7
3N/O	2.08(3)	1(3)					
1Imd	2.04(8)	7(7)					
1Imd	1.92(9)	2(10)					
1Imd	2.18(7)	6(5)	5(5)	0.2610	1649.528	152.764	9
2N/O	2.08(3)	4(3)					
1Imd	1.96(4)	17(3)					
1Imd	2.20(4)	15(2)					
1Imd	1.85(4)	11(4)					
1Imd	2.08(4)	18(3)	3(4)	0.2336	1475.877	167.754	11
1N/O							
1Imd							
1Imd							
1Imd							
1Imd							13

1Imd							
4N/O	2.10(3)	1(2)					
1Imd			6(4)	0.2705	1709.433	115.519	5
3N/O	2.09(3)	1(3)					
1Imd	2.19(6)	3(4)					
1Imd	2.03(6)	3(4)	7(4)	0.2765	1747.185	136.522	7
2N/O	2.08(3)	3(3)					
1Imd	2.08(6)	7(6)					
1Imd	2.21(5)	9(5)					
1Imd	2.08(5)	10(6)	7(4)	0.2913	1840.391	170.440	9
1N/O	2.08(3)	6(3)					
1Imd	1.87(4)	12(5)					
1Imd	1.98(4)	18(4)					
1Imd	2.09(4)	19(3)					
1Imd	2.21(4)	17(3)	5(4)	0.2751	1738.081	197.557	11
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			5(4)	0.2248	1334.606	196.356	11
3N/O	2.10(3)	1(3)					
1Imd	2.04(8)	0(6)	6(4)	0.3107	1963.546	132.691	5
2N/O	2.09(3)	2(3)					
1Imd	2.04(5)	4(3)					
1Imd	2.18(5)	5(3)	8(4)	0.3121	1971.830	154.075	7
1N/O	2.08(4)	6(3)					
1Imd	2.22(4)	12(4)					
1Imd	2.10(4)	13(4)					
1Imd	1.98(4)	10(4)	9(4)	0.3319	2097.492	194.251	9
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							9
2N/O	2.10(4)	1(4)					
1Imd	2.06(9)	0(7)	7(6)	0.3784	2390.964	161.575	5
1N/O							
1Imd			No Fit	No Fit	No Fit	No Fit	7

1Imd							
0N/O							
1Imd	2.06(2)	8(2)					
1Imd	1.94(2)	4(3)					
1Imd	2.18(2)	7(2)					7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	1.99(3)	4(1)					
1S	2.25(2)	4(1)					
1Imd	1.83(3)	4(2)	-7(4)	0.1558	984.304	76.912	7
3N/O	1.97(3)	7(1)					
1S	2.24(2)	5(1)					
1Imd	1.71(0.19)	15(3)					
1Imd	1.83(3)	6(2)	-10(5)	0.1591	1005.61	93.131	9
2N/O	2.02(5)	8(4)					
1S	2.27(3)	3(4)					
1Imd	2.09(8)	4(5)					
1Imd	1.92(8)	5(6)					
1Imd	2.78(7)	4(6)	-2(6)	0.1671	1056.16	120.048	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	1.99(3)	4(1)					
1S	2.25(2)	4(1)					
1Imd	1.83(3)	4(2)	-8(4)	0.1573	994.229	77.687	7
3N/O	1.97(3)	7(1)					
1S	2.23(2)	5(1)					
1Imd	1.83(3)	6(2)					
1Imd	1.72(0.15)	13(22)	-10(5)	0.1599	1010.467	93.58	9
2N/O	1.97(3)	11(2)					
1S	2.23(3)	6(2)					
1Imd	1.84(5)	8(3)					
1Imd	1.74(0.11)	1(11)					
1Imd	2.01(0.10)	4(6)	-10(6)	0.1807	1141.63	129.762	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	1.99(3)	4(1)					
1S	2.25(2)	4(1)					
1Imd	1.83(3)	4(2)	-8(5)	0.1591	1005.019	78.53	7
3N/O	1.97(2)	7(1)	-11(5)	0.1605	1014.39	93.944	9

1S	2.23(2)	5(1)					
1Imd	1.72(0.13)	11(19)					
1Imd	1.82(3)	6(2)					
2N/O	1.95(3)	10(2)					
1S	2.21(3)	6(2)					
1Imd	3.80(4)	6(4)					
1Imd	1.81(4)	6(2)					
1Imd	2.08(0.22)	10(4)	-14(8)	0.1666	1052.558	119.638	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	2(2)					
1S	2.65(2)	2(1)					
1Imd	2.01(4)	1(3)	8(3)	0.1313	829.924	64.849	7
3N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O	2.10(2)	9(1)					
1S	2.65(1)	4(1)					
1Imd	2.26(3)	11(2)					
1Imd	2.00(2)	11(2)					
1Imd	2.13(3)	13(2)	11(2)	0.0972	614.108	69.802	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	2(2)					
1S	2.65(2)	2(1)					
1Imd	2.01(4)	2(3)	7(3)	0.1285	811.923	63.442	7
3N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O							
1S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)	5(5)	0.1875	1184.791	92.577	7

1Br	2.42(2)	3(2)					
1Imd	2.12(0.22)	10(27)					
2N/O	2.06(3)	4(2)					
1Br	2.42(3)	3(2)					
1Imd	1.99(8)	1(6)					
1Imd	2.17(6)	2(5)	5(5)	0.1950	1232.112	114.107	9
1N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)					
1Br	2.42(2)	3(2)					
1Imd	2.13(0.20)	9(26)	6(4)	0.1831	1156.819	90.392	7
2N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.07(2)	8(2)					
1Br	2.42(2)	1(2)					
1Imd	2.29(5)	10(3)					
1Imd	2.02(4)	9(3)					
1Imd	2.15(4)	12(3)	10(3)	0.1672	1056.515	120.088	11

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)					
1Br	2.42(2)	3(2)					
1Imd	2.13(0.19)	9(25)	6(4)	0.1794	1133.834	88.596	7
2N/O	2.07(3)	4(2)					
1Br	2.42(3)	3(2)					
1Imd	2.18(6)	2(5)					
1Imd	2.00(8)	0(6)	6(5)	0.1868	1180.547	109.332	9
1N/O	2.07(2)	8(2)					
1Br	1.43(2)	1(2)					
1Imd	2.02(4)	9(3)					
1Imd	2.15(4)	12(3)					
1Imd	2.29(4)	10(3)	10(3)	0.1627	1027.907	116.836	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(1)	4(1)					
1Br	2.75(1)	1(1)					
1Imd	1.98(2)	6(1)	4(3)	0.0879	555.226	43.384	7
2N/O	2.11(2)	5(1)					
1Br	2.76(2)	1(1)					
1Imd	2.11(4)	3(5)					
1Imd	1.98(2)	7(1)	5(3)	0.0938	592.795	54.899	9
1N/O	2.11(2)	9(2)					
1Br	2.76(2)	1(1)					
1Imd	1.97(2)	12(2)					
1Imd	2.09(3)	13(2)					
1Imd	2.22(3)	1(3)	7(2)	0.1082	683.754	77.718	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(3)	5(2)					
2S	2.22(3)	1(1)					
1Imd	1.80(3)	4(2)	-12(5)	0.1644	1038.536	81.149	7
1N/O	1.93(3)	9(2)					
2S	2.20(2)	2(1)					
1Imd	1.70(0.13)	11(19)					
1Imd	1.80(3)	6(2)	-16(5)	0.1624	1026.497	95.065	9
0N/O							
2S	2.15(4)	2(3)					
1Imd	1.75(8)	4(6)					
1Imd	1.90(0.12)	5(7)					
1Imd	2.06(0.13)	3(10)	-22(11)	0.3233	2043.186	189.222	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	7(1)					
2S	2.23(2)	5(1)					
1Imd	1.82(3)	5(2)	-10(5)	0.1636	1033.515	80.757	7
1N/O	1.94(3)	10(2)					
2S	2.20(3)	6(1)					
1Imd	2.05(0.15)	7(22)					
1Imd	1.80(4)	7(2)	-15(7)	0.1877	1185.834	109.821	9
0N/O							
2S	2.25(5)	1(5)					
1Imd	1.93(0.20)	1(22)					
1Imd	2.03(0.13)	6(11)					
1Imd	2.15(0.19)	4(17)	0(10)	0.4233	2674.9	247.725	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.95(3)	5(2)					
2S	2.21(3)	1(1)					
1Imd	1.80(3)	4(2)	-14(5)	0.1658	1047.874	81.879	7
1N/O	1.93(3)	9(1)					
2S	2.19(2)	2(1)					
1Imd	1.71(0.11)	8(16)					
1Imd	1.79(3)	6(2)	-18(5)	0.1595	1007.715	93.325	9
0N/O							
2S	2.15(4)	2(3)					
1Imd	1.74(8)	4(5)					
1Imd	2.06(0.13)	3(10)					
1Imd	1.89(0.12)	5(7)	-23(11)	0.3121	1972.015	182.63	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(3)	1(3)					
2S	2.65(2)	2(2)					
1Imd	2.06(5)	1(4)	10(3)	0.2032	1283.757	100.31	7
1N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
2S	2.67(2)	2(3)					
1Imd	2.14(3)	14(3)					
1Imd	2.26(3)	12(3)					
1Imd	2.02(2)	13(2)	13(2)	0.2508	1584.943	146.783	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(3)	1(3)					
2S	2.65(2)	2(2)					
1Imd	2.06(5)	1(4)	9(3)	0.2000	1264.062	98.771	7
1N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	3(2)	7(5)	0.2410	1522.855	118.993	7

2Br	2.42(3)	7(2)					
1Imd	2.17(9)	1(10)					
1N/O	2.07(3)	6(3)					
2Br	2.42(3)	7(3)					
1Imd	2.05(8)	2(7)					
1Imd	2.20(5)	4(5)	9(4)	0.2523	1594.262	147.646	9
0N/O							
2Br	2.42(3)	6(3)					
1Imd	2.16(3)	15(3)					
1Imd	2.04(2)	13(2)					
1Imd	2.29(3)	13(3)	14(3)	0.2733	1726.725	159.914	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	3(2)					
2Br	2.42(3)	7(2)					
1Imd	2.17(8)	1(9)	7(5)	0.2352	1486.355	116.141	7
1N/O							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
2Br	2.42(3)	6(3)					
1Imd	2.16(3)	15(2)					
1Imd	2.04(2)	13(2)					
1Imd	2.29(3)	13(3)	14(3)	0.2663	1682.515	155.819	11

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	3(2)					
2Br	2.42(3)	7(2)					
1Imd	2.18(8)	1(9)	7(5)	0.2303	1455.022	113.693	7
1N/O	2.07(3)	5(3)					
2Br	2.42(3)	8(3)					
1Imd	2.20(5)	4(5)					
1Imd	2.06(7)	2(6)	9(4)	0.2401	1517.318	140.52	9
0N/O							
2Br	2.42(3)	6(3)					
1Imd	2.29(3)	13(3)					
1Imd	2.04(2)	13(2)					
1Imd	2.16(3)	15(2)	14(3)	0.2604	1645.601	152.401	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(1)					
2Br	2.76(2)	4(1)					
1Imd	1.99(3)	6(1)	4(4)	0.1588	1003.162	78.385	7
1N/O	2.12(3)	7(3)					
2Br	2.77(2)	3(2)					
1Imd	1.99(2)	8(2)					
1Imd	2.12(3)	6(3)	6(3)	0.1551	980.115	90.769	9
0N/O							
2Br	2.80(2)	5(2)					
1Imd	2.00(2)	12(3)					
1Imd	2.11(3)	14(3)					
1Imd	2.22(3)	12(4)	10(3)	0.2401	1516.968	140.488	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.00(3)	2(1)					
1S	2.26(3)	3(2)					
1Imd	1.83(3)	3(2)	-6(4)	0.1596	1008.578	78.808	7
3N/O	1.99(2)	5(1)					
1S	2.25(2)	5(1)					
1Imd	1.84(3)	5(2)					
1Imd	1.76(8)	6(13)	-8(4)	0.1476	932.919	86.399	9
2N/O	1.98(4)	7(2)					
1S	2.24(4)	5(2)					
1Imd	1.66(0.13)	2(10)					
1Imd	1.44(0.12)	5(11)					
1Imd	1.83(4)	6(2)	-9(7)	0.1451	916.923	104.221	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.00(3)	2(1)					
1S	2.26(3)	3(2)					
1Imd	1.82(3)	2(2)	-7(4)	0.1610	1017.618	79.515	7
3N/O	1.99(2)	5(1)					
1S	2.25(2)	4(1)					
1Imd	1.83(3)	4(2)					
1Imd	1.75(7)	5(11)	-9(4)	0.1489	940.570	87.107	9
2N/O	1.98(4)	7(2)					
1S	2.24(4)	5(2)					
1Imd	1.64(0.13)	3(10)					
1Imd	1.42(0.10)	4(11)					
1Imd	1.82(3)	5(2)	-10(7)	0.1447	914.410	103.936	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	1(1)					
1S	2.64(2)	2(1)					
1Imd	2.00(2)	2(1)	7(2)	0.0958	605.087	47.280	7
3N/O	2.09(1)	2(1)					
1S	2.65(1)	2(1)					
1Imd	2.18(3)	3(2)					
1Imd	1.99(1)	2(1)	8(2)	0.0886	560.134	51.875	9
2N/O	2.10(1)	5(1)					
1S	2.65(1)	4(1)					
1Imd	2.00(3)	9(3)					
1Imd	2.27(3)	11(2)					
1Imd	2.14(1)	4(1)	10(2)	0.0729	460.634	52.358	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.13(2)	3(2)					
1N/O	2.01(2)	6(3)					
1S	2.64(2)	1(2)					
1Imd	2.03(2)	0(2)	7(2)	0.0906	572.708	53.039	9
2N/O	2.05(2)	4(2)					
2N/O	2.17(2)	4(3)					
1S	2.64(2)	1(2)					
1Imd	2.03(2)	1(2)	7(2)	0.0821	518.688	48.036	9
1N/O	2.02(3)	5(3)					
3N/O	2.14(2)	2(3)					
1S	2.64(2)	1(2)					
1Imd	2.02(2)	1(2)	6(2)	0.0834	527.062	48.812	9
2N/O	2.08(1)	10(1)					
1N/O	2.23(2)	12(2)					
1S	2.60(2)	3(2)					
1Imd	1.94(2)	8(1)					
1Imd	2.11(2)	3(2)	7(1)	0.0354	223.731	25.300	11
1N/O	2.04(1)	13(1)					
2N/O	2.19(2)	9(2)					
1S	2.60(2)	3(2)					
1Imd	1.94(2)	9(1)					
1Imd	2.10(2)	3(2)	7(1)	0.0319	201.818	22.939	11
1N/O							
1N/O							
1S			No Fit	No Fit	No Fit	No Fit	13

1Imd							
1Imd							
1Imd							

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.01(3)	0(1)					
1S	2.27(3)	2(2)					
1Imd	1.82(3)	2(3)	-6(4)	0.1690	1067.621	83.422	7
4N/O	2.00(2)	3(1)					
1S	2.26(2)	4(2)					
1Imd	1.76(6)	2(11)					
1Imd	1.84(4)	4(3)	-8(4)	0.1465	925.951	85.753	9
3N/O	1.99(3)	5(2)					
1S	2.25(3)	4(2)					
1Imd	1.84(4)	5(2)					
1Imd	1.72(0.10)	1(12)					
1Imd	1.48(0.15)	7(14)	-8(6)	0.1359	859.005	97.638	11
2N/O	1.98(4)	7(2)					
1S	2.25(4)	5(2)					
1Imd	1.64(0.18)	3(16)					
1Imd	1.81(0.20)	6(10)					
1Imd	1.46(0.15)	2(15)					
1Imd	1.88(0.22)	1(50)	-9(8)	0.1407	889.223	130.809	13

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.01(3)	0(2)					
1S	2.27(3)	2(2)					
1Imd	1.82(3)	2(3)	-6(4)	0.1699	1073.709	83.898	7
4N/O	2.00(2)	3(1)					
1S	2.26(2)	3(2)					
1Imd	1.84(5)	4(3)					
1Imd	1.76(6)	2(11)	-8(4)	0.1476	932.701	86.378	9
3N/O	1.99(3)	5(2)					
1S	2.25(3)	4(2)					
1Imd	1.83(4)	5(3)					
1Imd	1.72(0.10)	1(12)					
1Imd	1.48(0.15)	7(14)	-9(6)	0.1363	861.030	97.868	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.01(3)	0(2)	-6(4)	0.1710	1080.713	84.445	7

1S	2.27(3)	2(2)					
1Imd	1.82(3)	2(3)					
4N/O	1.99(2)	3(1)					
1S	2.26(2)	3(2)					
1Imd	1.84(5)	4(3)					
1Imd	1.76(5)	1(10)	-8(4)	0.1486	938.814	86.944	9
3N/O	1.99(3)	5(2)					
1S	2.25(3)	4(2)					
1Imd	1.47(0.15)	7(14)					
1Imd	1.71(0.10)	1(12)					
1Imd	1.83(4)	5(3)	-9(6)	0.1368	864.297	98.240	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.10(1)	1(1)					
1S	2.64(1)	1(1)					
1Imd	2.00(4)	1(4)	6(2)	0.0860	543.196	42.444	7
4N/O	2.10(1)	1(1)					
1S	2.64(1)	2(1)					
1Imd	1.99(3)	2(3)					
1Imd	2.19(5)	1(6)	7(2)	0.0815	515.008	47.695	9
3N/O	2.10(1)	3(1)					
1S	2.65(1)	3(1)					
1Imd	2.29(4)	7(3)					
1Imd	2.15(4)	9(3)					
1Imd	2.00(3)	7(2)	9(2)	0.0699	441.693	50.205	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.10(1)	1(1)					
1S	2.64(1)	1(1)					
1Imd	2.00(4)	1(4)	6(2)	0.0834	526.817	41.164	7
4N/O	2.10(1)	1(1)					
1S	2.64(1)	2(1)					
1Imd	2.19(5)	1(6)					
1Imd	1.99(3)	2(3)	7(2)	0.0790	499.166	46.228	9
3N/O	2.10(1)	3(1)					
1S	2.65(1)	3(1)					
1Imd	2.15(4)	9(2)					
1Imd	2.29(4)	7(3)					
1Imd	2.00(3)	7(2)	9(2)	0.0677	427.865	48.633	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	7(1)	7(1)	0.0355	224.452	25.512	9
1N/O	2.26(2)	10(2)					
1S	2.61(2)	3(2)					
1Imd	2.11(2)	6(2)					
1Imd	1.95(2)	8(1)					
2N/O	2.07(1)	9(1)	7(1)	0.0324	204.827	23.281	9
2N/O	2.22(2)	7(2)					
1S	2.61(2)	3(1)					
1Imd	1.94(2)	8(1)					
1Imd	2.11(2)	7(1)					
1N/O	2.04(2)	11(1)	7(1)	0.0330	208.709	23.723	9
3N/O	2.19(2)	4(2)					
1S	2.61(2)	3(1)					
1Imd	2.10(2)	7(1)					
1Imd	1.94(2)	9(1)					
2N/O	2.17(2)	9(3)	7(2)	0.0444	280.274	41.230	11
1N/O	2.03(2)	13(2)					
1S	2.61(3)	2(3)					
1Imd	2.10(3)	10(2)					
1Imd	1.94(3)	10(2)					
1Imd	2.25(5)	5(4)					
1N/O	2.04(2)	13(1)	6(2)	0.0294	185.958	27.355	11
2N/O	2.19(2)	9(2)					
1S	2.60(2)	4(2)					
1Imd	2.10(2)	9(1)					
1Imd	2.63(0.12)	6(17)					
1Imd	1.94(2)	10(1)					
0N/O			8(2)	0.0782	494.166	56.169	11
3N/O	2.10(1)	3(1)					
1S	2.64(2)	3(1)					
1Imd	2.29(4)	7(3)					
1Imd	2.15(4)	9(3)					
1Imd	2.00(3)	7(2)					

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.06(2)	1(1)					
1Br	2.40(2)	4(2)					
1Imd	1.88(7)	4(8)	1(4)	0.1594	1007.237	78.704	7
4N/O	2.07(3)	0(2)					
1Br	2.41(3)	4(2)					
1Imd	1.97(0.14)	5(14)	4(5)	0.1615	1020.718	94.530	9

1Imd	2.23(0.11)	2(10)					
3N/O	2.07(2)	2(2)					
1Br	2.42(3)	2(2)					
1Imd	2.30(8)	6(5)					
1Imd	2.01(9)	3(6)					
1Imd	2.16(8)	7(5)	7(4)	0.1585	1001.772	113.866	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.06(2)	1(1)					
1Br	2.41(2)	4(2)					
1Imd	1.88(7)	5(9)	1(4)	0.1567	990.274	77.378	7
4N/O	2.08(3)	0(2)					
1Br	2.42(2)	4(2)					
1Imd	2.24(0.11)	2(9)					
1Imd	2.00(0.16)	6(15)	5(4)	0.1571	992.895	91.953	9
3N/O	2.07(2)	2(2)					
1Br	2.42(3)	2(2)					
1Imd	2.30(7)	7(5)					
1Imd	2.01(8)	3(6)					
1Imd	2.17(7)	7(5)	7(4)	0.1531	967.293	109.946	11

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.06(2)	1(1)					
1Br	2.41(2)	4(2)					
1Imd	1.89(7)	5(10)	1(4)	0.1544	975.874	76.253	7
4N/O	2.08(3)	0(2)					
1Br	2.42(2)	4(2)					
1Imd	2.25(0.10)	1(8)					
1Imd	2.02(0.17)	6(15)	6(4)	0.1534	969.583	89.794	9
3N/O	2.08(2)	2(2)					
1Br	2.42(3)	2(2)					
1Imd	2.17(7)	7(5)					
1Imd	2.30(7)	7(5)					
1Imd	2.01(8)	3(5)	7(3)	0.1487	939.905	106.833	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	7

4N/O	2.10(1)	2(1)					
1Br	2.75(1)	1(1)					
1Imd	2.07(0.14)	11(17)					
1Imd	1.97(2)	5(1)	4(2)	0.0608	384.464	35.606	9
3N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	1.99(3)	0(2)					
2S	2.24(3)	2(2)					
1Imd	1.80(3)	1(3)	-9(5)	0.1787	1129.253	88.238	7
3N/O	1.97(3)	3(2)					
2S	2.23(2)	0(2)					
1Imd	1.74(5)	0(8)					
1Imd	1.83(5)	4(3)	-11(4)	0.1548	978.223	90.594	9
2N/O	1.96(3)	5(2)					
2S	2.23(3)	1(2)					
1Imd	1.44(0.13)	5(12)					
1Imd	1.68(0.14)	2(13)					
1Imd	1.81(4)	5(2)	-12(6)	0.1388	876.854	99.667	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	1.99(3)	0(2)					
2S	2.24(3)	2(2)					
1Imd	1.80(3)	1(3)	-9(5)	0.1797	1135.518	88.727	7
3N/O	1.97(3)	3(2)					
2S	2.23(2)	0(2)					
1Imd	1.74(4)	1(8)					
1Imd	1.83(5)	4(3)	-12(4)	0.1554	982.004	90.944	9
2N/O	1.96(3)	4(2)					
2S	2.22(3)	0(2)					
1Imd	1.81(4)	5(3)					
1Imd	1.43(0.13)	5(12)					
1Imd	1.68(0.14)	3(13)	-12(6)	0.1390	878.628	99.869	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	1.99(3)	1(2)					
2S	2.24(3)	2(2)	-10(5)	0.1805	1140.636	89.127	7

1Imd	1.80(4)	1(2)					
3N/O	1.96(3)	3(2)					
2S	2.22(2)	0(2)					
1Imd	1.73(4)	1(7)					
1Imd	1.83(5)	4(3)	-13(4)	0.1555	982.819	91.020	9
2N/O	1.96(3)	5(2)					
2S	2.22(3)	0(2)					
1Imd	1.68(0.15)	3(14)					
1Imd	1.81(4)	5(3)					
1Imd	1.42(0.13)	5(13)	-1(60	0.1392	879.430	99.960	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.11(2)	1(2)					
2S	2.65(2)	2(1)					
1Imd	2.04(4)	0(3)	8(2)	0.1063	671.620	52.479	7
3N/O	2.10(2)	1(2)					
2S	2.65(2)	2(2)					
1Imd	2.20(4)	2(3)					
1Imd	2.03(4)	2(3)	9(2)	0.0988	623.991	57.788	9
2N/O	2.10(2)	4(2)					
2S	2.65(1)	1(1)					
1Imd	2.01(2)	10(2)					
1Imd	2.27(3)	10(2)					
1Imd	2.14(3)	12(2)	11(2)	0.0820	517.946	58.872	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.11(2)	1(2)					
2S	2.65(2)	3(1)					
1Imd	2.04(4)	0(3)	8(2)	0.1036	654.627	51.151	7
3N/O	2.10(2)	1(2)					
2S	2.65(2)	2(2)					
1Imd	2.20(4)	2(3)					
1Imd	2.03(4)	2(2)	9(2)	0.0963	608.280	56.333	9
2N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
2Br	2.41(2)	8(2)					
1Imd	2.24(6)	0(5)	6(3)	0.1832	1157.481	90.443	7
3N/O	2.09(3)	0(3)					
2Br	2.41(3)	8(3)					
1Imd	2.07(8)	0(7)					
1Imd	2.25(6)	2(4)	8(3)	0.1809	1143.310	105.883	9
2N/O	2.09(3)	2(3)					
2Br	2.41(3)	6(3)					
1Imd	2.03(4)	8(4)					
1Imd	2.16(4)	11(3)					
1Imd	2.29(4)	10(3)	10(1)	0.1691	1068.431	121.442	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
2Br	2.41(2)	8(2)					
1Imd	2.24(6)	0(5)	7(3)	0.1770	1118.608	87.406	7
3N/O	2.09(3)	0(3)					
2Br	2.41(3)	8(3)					
1Imd	2.25(6)	2(4)					
1Imd	2.07(8)	0(7)	8(3)	0.1743	1101.206	101.984	9
2N/O	2.09(3)	2(3)					
2Br	2.41(3)	6(3)					
1Imd	2.16(5)	12(3)					
1Imd	2.03(5)	9(3)					
1Imd	2.29(4)	11(3)	10(3)	0.1612	1018.508	115.768	11

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
2Br	2.42(2)	8(2)					
1Imd	2.24(6)	0(5)	7(3)	0.1720	1086.566	84.902	7
3N/O	2.09(3)	0(3)					
2Br	2.42(2)	8(3)					
1Imd	2.25(5)	2(4)					
1Imd	2.07(8)	0(7)	8(3)	0.1688	1066.784	98.796	9
2N/O	2.09(3)	2(3)					
2Br	2.41(3)	6(3)					
1Imd	2.16(4)	12(3)					
1Imd	2.29(4)	11(3)					
1Imd	2.03(5)	9(3)	10(3)	0.1548	978.206	111.187	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O							
2Br							
1Imd			No Fit	No Fit	No Fit	No Fit	7
3N/O	2.11(2)	2(1)					
2Br	2.76(1)	4(1)					
1Imd	2.10(4)	2(5)					
1Imd	1.98(2)	5(2)	5(2)	0.0697	440.331	40.779	9
2N/O	2.12(2)	4(2)					
2Br	2.77(1)	4(1)					
1Imd	2.21(4)	8(4)					
1Imd	1.96(2)	10(2)					
1Imd	2.08(3)	11(3)	7(2)	0.0793	500.842	56.928	11

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.47(2)	10(1)					
1Br	2.42(2)	7(1)					
1Imd	1.94(4)	1(5)	4(2)	0.0612	352.139	32.612	9
3N/O	2.07(1)	5(1)					
1S	2.47(2)	12(1)					
1Br	2.42(2)	8(1)					
1Imd	2.23(8)	3(10)					
1Imd	1.97(4)	2(3)	5(2)	0.0512	323.786	36.803	11
2N/O	2.08(2)	6(2)					
1S	2.48(3)	12(2)					
1Br	2.43(3)	8(2)					
1Imd	2.00(4)	6(3)					
1Imd	2.82(6)	4(4)					
1Imd	2.19(6)	0(7)	7(2)	0.0392	247.974	36.478	13

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	3(1)					
1S	2.47(2)	10(1)					
1Br	2.43(2)	7(1)					
1Imd	1.95(4)	0(5)	4(2)	0.0563	355.719	32.944	9
3N/O	2.07(1)	5(1)					
1S	2.47(2)	12(1)					
1Br	2.43(2)	8(1)	6(2)	0.0461	291.235	33.103	11

1Imd	1.98(4)	3(3)					
1Imd	2.22(7)	2(8)					
2N/O	2.08(2)	6(2)					
1S	2.47(3)	12(2)					
1Br	2.43(3)	8(2)					
1Imd	2.00(4)	6(3)					
1Imd	2.81(6)	4(5)					
1Imd	2.18(6)	1(6)	7(2)	0.036	227.265	33.432	13

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	2(1)					
1S	2.47(2)	10(1)					
1Br	2.43(2)	6(1)					
1Imd	1.96(4)	0(4)	4(2)	0.0546	344.736	31.926	9
3N/O	2.07(1)	5(1)					
1S	2.47(2)	11(1)					
1Br	2.43(2)	8(1)					
1Imd	2.21(6)	1(7)					
1Imd	1.98(3)	3(3)	6(2)	0.0442	279.593	31.780	11
2N/O	2.09(2)	6(2)					
1S	2.47(3)	12(2)					
1Br	2.43(3)	8(2)					
1Imd	2.81(6)	4(4)					
1Imd	2.17(5)	2(5)					
1Imd	2.00(3)	7(2)	7(2)	0.0353	222.771	32.771	13

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(1)	2(1)					
1S	2.48(0.11)	14(13)					
1Br	2.75(1)	0(1)					
1Imd	1.97(2)	5(1)	5(2)	0.0522	330.026	30.564	9
3N/O	2.11(2)	3(1)					
1S	2.51(9)	10(11)					
1Br	2.76(2)	0(1)					
1Imd	1.98(2)	6(1)					
1Imd	2.10(5)	1(6)	6(2)	0.0517	326.478	37.109	11
2N/O	2.08(3)	6(2)					
1S	2.36(7)	3(10)					
1Br	2.72(3)	1(2)					
1Imd	1.95(4)	7(2)					
1Imd	2.08(8)	3(9)	1(4)	0.0685	432.772	63.663	13

1Imd	1.88(0.17)	7(24)					

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.47(2)	11(1)					
1Br	2.42(2)	7(1)					
1Imd	1.93(4)	2(5)	3(2)	0.0584	368.897	34.164	9
3N/O	2.06(1)	5(1)					
1S	2.47(2)	12(1)					
1Br	2.42(2)	9(1)					
1Imd	2.25(0.10)	5(13)					
1Imd	1.97(4)	2(4)	5(2)	0.0487	307.633	34.967	11
2N/O	2.07(2)	6(2)					
1S	2.48(3)	13(2)					
1Br	2.43(3)	9(2)					
1Imd	2.82(7)	3(5)					
1Imd	2.20(8)	2(10)					
1Imd	2.00(5)	5(3)	6(2)	0.0372	235.142	34.591	13

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.47(2)	11(1)					
1Br	2.43(2)	7(1)					
1Imd	1.94(4)	2(5)	3(2)	0.0530	334.619	30.989	9
3N/O	2.07(1)	5(1)					
1S	2.47(2)	12(1)					
1Br	2.43(2)	8(1)					
1Imd	2.24(9)	5(11)					
1Imd	1.98(4)	2(3)	5(2)	0.0435	274.802	31.235	11
2N/O	2.07(2)	6(2)					
1S	2.48(3)	13(2)					
1Br	2.43(3)	9(2)					
1Imd	2.18(6)	1(7)					
1Imd	2.00(4)	6(3)					
1Imd	2.81(7)	3(5)	6(2)	0.0337	212.846	31.311	13

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	3(1)					
1S	2.48(2)	11(1)	4(2)	0.0512	323.248	29.936	9

1Br	2.43(2)	7(1)					
1Imd	1.95(4)	1(5)					
3N/O	2.07(1)	5(1)					
1S	2.48(2)	12(1)					
1Br	2.43(2)	8(1)					
1Imd	1.98(4)	3(3)					
1Imd	2.22(7)	3(9)	5(2)	0.0417	263.721	29.976	11
2N/O	2.08(2)	6(2)					
1S	2.48(3)	12(2)					
1Br	2.43(3)	9(2)					
1Imd	2.00(4)	6(3)					
1Imd	2.81(6)	4(5)					
1Imd	2.17(6)	1(6)	6(2)	0.0327	206.915	30.438	13

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(1)	2(1)					
1S	2.50(0.10)	14(13)					
1Br	2.75(1)	0(1)					
1Imd	1.97(2)	5(1)	5(2)	0.0514	324.486	30.051	9
3N/O	2.11(2)	3(1)					
1S	2.52(8)	10(11)					
1Br	2.76(2)	0(1)					
1Imd	2.10(5)	1(6)					
1Imd	1.98(2)	6(1)	6(2)	0.0508	320.729	36.455	11
2N/O	2.12(2)	4(2)					
1S	2.59(5)	2(7)					
1Br	2.78(3)	1(2)					
1Imd	2.23(4)	9(3)					
1Imd	1.97(3)	11(2)					
1Imd	2.09(3)	12(2)	8(2)	0.0562	355.114	52.239	13

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.05(1)	3(1)					
1S	2.47(2)	11(1)					
1Br	2.41(2)	8(1)					
1Imd	1.92(4)	1(4)	2(2)	0.0547	345.749	32.020	9
3N/O	2.07(1)	4(1)					
1S	2.49(3)	11(2)					
1Br	2.43(2)	8(2)					
1Imd	2.01(5)	1(5)					
1Imd	2.82(4)	4(4)	5(2)	0.0362	229.053	26.035	11

2N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.47(2)	11(1)					
1Br	2.42(1)	7(1)					
1Imd	1.93(4)	1(5)	3(2)	0.0489	309.059	28.622	9
3N/O	2.06(1)	5(1)					
1S	2.47(2)	12(1)					
1Br	2.42(2)	8(1)					
1Imd	1.97(4)	1(3)					
1Imd	2.24(0.13)	10(20)	5(2)	0.0408	258.017	29.327	11
2N/O	2.06(2)	7(1)					
1S	2.47(2)	13(1)					
1Br	2.42(2)	9(1)					
1Imd	2.29(0.47)	27(225)					
1Imd	2.16(0.16)	2(14)					
1Imd	1.97(3)	4(5)	5(3)	0.0394	249.041	36.635	13

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.48(2)	11(1)					
1Br	2.43(1)	7(1)					
1Imd	1.94(4)	1(5)	3(2)	0.0463	292.688	27.106	9
3N/O	2.07(1)	5(1)					
1S	2.48(2)	12(1)					
1Br	2.43(2)	8(1)					
1Imd	1.97(4)	2(3)					
1Imd	2.23(0.10)	8(14)	5(2)	0.0385	242.987	27.619	11
2N/O	2.08(2)	6(2)					
1S	2.48(3)	13(2)					
1Br	2.43(2)	9(1)					
1Imd	2.17(7)	2(8)					
1Imd	1.99(4)	6(3)					
1Imd	2.80(6)	4(5)	6(2)	0.03	189.462	27.871	13

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(1)	2(1)					
1S	2.51(0.10)	14(13)					
1Br	2.75(1)	0(1)					
1Imd	1.98(2)	5(1)	5(2)	0.0506	319.614	29.600	9
3N/O	2.11(2)	3(1)					
1S	2.53(8)	10(11)					
1Br	2.76(2)	0(1)					
1Imd	1.98(2)	6(1)					
1Imd	2.10(5)	1(6)	6(2)	0.0500	316.236	35.945	11
2N/O	2.12(2)	4(2)					
1S	2.59(6)	3(7)					
1Br	2.78(3)	1(2)					
1Imd	2.09(3)	12(2)					
1Imd	1.97(3)	11(2)					
1Imd	2.23(4)	9(3)	8(2)	0.0558	352.408	51.841	13

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.05(1)	3(1)					
1S	2.47(2)	11(1)					
1Br	2.41(2)	7(1)					
1Imd	1.91(3)	1(4)	2(2)	0.0537	339.503	31.442	9
3N/O	2.05(1)	5(1)					
1S	2.47(2)	12(1)					
1Br	2.41(2)	8(1)					
1Imd	1.94(4)	1(4)					
1Imd	2.25(0.26)	20(55)	3(2)	0.0466	294.158	33.435	11
2N/O	2.05(2)	9(2)					
1S	2.50(4)	15(4)					
1Br	2.44(3)	11(4)					
1Imd	1.92(4)	7(4)					
1Imd	2.07(5)	10(6)					
1Imd	2.24(6)	7(7)	5(2)	0.0461	291.594	42.895	13

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.47(2)	11(1)					
1Br	2.42(1)	7(1)					
1Imd	1.92(3)	1(4)	3(2)	0.0480	303.492	28.107	9

3N/O	2.06(1)	5(1)					
1S	2.47(2)	12(1)					
1Br	2.42(1)	8(1)					
1Imd	1.95(4)	1(4)					
1Imd	2.23(0.21)	17(37)	4(2)	0.0417	263.578	29.959	11
2N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.47(2)	11(1)					
1Br	2.42(1)	7(1)					
1Imd	1.93(3)	1(4)	3(2)	0.0451	284.701	26.366	9
3N/O	2.06(1)	5(1)					
1S	2.48(2)	12(1)					
1Br	2.43(1)	8(1)					
1Imd	1.96(4)	1(3)					
1Imd	2.22(0.15)	12(22)	4(2)	0.0391	247.133	28.090	11
2N/O	2.06(2)	7(1)					
1S	2.47(2)	12(2)					
1Br	2.42(2)	8(2)					
1Imd	2.14(0.10)	0(14)					
1Imd	2.31(0.30)	20(137)					
1Imd	1.96(3)	5(5)	5(3)	0.039	246.405	36.247	13

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	2(1)					
1S	2.49(2)	9(2)					
1Br	2.44(2)	6(2)					
1Imd	2.86(3)	3(3)	5(1)	0.0367	231.892	21.476	9
3N/O	2.11(2)	3(1)					
1S	2.54(8)	10(11)					
1Br	2.76(2)	0(1)					
1Imd	1.98(2)	6(1)					
1Imd	2.10(5)	1(6)	6(2)	0.0494	312.322	35.500	11
2N/O	2.12(2)	4(2)					
1S	2.60(6)	3(7)	8(2)	0.0553	349.613	51.43	13

1Br	2.78(3)	1(2)					
1Imd	2.09(3)	12(2)					
1Imd	2.23(4)	9(3)					
1Imd	1.97(3)	11(2)					

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(3)	4(2)					
1S	2.62(3)	4(2)					
1Br	2.17(6)	4(5)					
1Imd	1.95(3)	5(2)	5(3)	0.0777	491.244	45.495	9
3N/O	2.09(2)	8(1)					
1S	2.62(2)	6(1)					
1Br	2.19(3)	2(2)					
1Imd	2.12(2)	7(1)					
1Imd	1.96(2)	9(1)	6(1)	0.0326	206.273	23.446	11
2N/O	2.05(2)	9(2)					
1S	2.50(5)	14(4)					
1Br	2.44(4)	11(3)					
1Imd	1.92(4)	8(3)					
1Imd	2.25(6)	7(6)					
1Imd	2.08(5)	10(5)	5(3)	0.0439	277.505	40.823	13

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.05(1)	3(1)					
1S	2.47(2)	10(1)					
1Br	2.42(2)	7(1)					
1Imd	1.91(3)	0(3)	2(2)	0.0489	308.954	28.613	9
3N/O	2.06(1)	5(1)					
1S	2.47(2)	11(1)					
1Br	2.42(1)	8(1)					
1Imd	2.23(0.27)	22(56)					
1Imd	1.94(3)	2(3)	3(2)	0.0423	267.473	30.402	11
2N/O	2.06(2)	8(2)					
1S	2.50(5)	14(4)					
1Br	2.44(4)	10(3)					
1Imd	1.92(5)	7(4)					
1Imd	2.23(7)	6(6)					
1Imd	2.07(7)	9(6)	5(3)	0.0421	266.093	39.144	13

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	3(1)					
1S	2.47(2)	10(1)					
1Br	2.42(1)	7(1)					
1Imd	1.92(3)	0(4)	2(2)	0.0455	287.196	26.598	9
3N/O	2.06(1)	5(1)					
1S	2.47(2)	11(1)					
1Br	2.42(1)	8(1)					
1Imd	1.95(3)	2(3)					
1Imd	2.21(0.20)	17(34)	4(2)	0.0394	249.247	28.330	11
2N/O	2.06(2)	8(1)					
1S	2.49(4)	13(3)					
1Br	2.43(4)	10(3)					
1Imd	2.22(8)	6(7)					
1Imd	1.92(5)	7(4)					
1Imd	2.06(7)	9(6)	5(3)	0.0404	255.062	37.521	13

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(1)	2(1)					
1S	2.52(9)	14(13)					
1Br	2.75(1)	0(1)					
1Imd	1.98(2)	5(1)	5(2)	0.0493	311.473	28.846	9
3N/O	2.11(2)	3(1)					
1S	2.54(8)	10(10)					
1Br	2.76(2)	0(1)					
1Imd	1.98(2)	6(1)					
1Imd	2.10(5)	1(6)	6(2)	0.0489	308.700	35.088	11
2N/O	2.12(2)	4(2)					
1S	2.60(6)	3(7)					
1Br	2.78(3)	1(2)					
1Imd	2.23(4)	9(3)					
1Imd	1.97(3)	11(2)					
1Imd	2.09(3)	12(2)	8(2)	0.0545	344.271	50.644	13

Table F.3. Additional Fits for Co(II) E34A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(3)	2(2)	neg1(7)	0.2723	858.336	126.284	3
3N/O	2.11(2)	4(2)	neg1(4)	0.1548	487.934	71.788	3

4N/O	2.11(2)	5(1)	neg1(3)	0.0920	290.010	42.668	3
5N/O	2.11(1)	7(1)	neg2(2)	0.0637	200.846	29.550	3
6N/O	2.11(1)	9(1)	neg2(2)	0.0577	181.825	26.751	3
7N/O	2.10(2)	10(1)	neg3(2)	0.0657	207.138	30.476	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.20(4)	6(2)	neg22(9)	0.2438	768.514	113.069	3
3S	2.20(3)	8(2)	neg22(6)	0.1678	528.860	77.809	3
4S	2.21(3)	11(1)	neg22(5)	0.1325	417.776	61.466	3
5S	2.21(3)	12(1)	neg22(5)	0.1182	372.554	54.813	3
6S	2.21(3)	14(2)	neg22(5)	0.1152	363.048	53.414	3
7S	2.21(3)	16(2)	neg22(5)	0.1184	373.388	54.935	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.05(2)	1(2)					
1N/O	2.18(2)	4(2)	neg2(4)	0.0855	269.646	56.213	5
2N/O	2.04(2)	1(2)					
2N/O	2.17(2)	1(2)	neg2(2)	0.0520	163.981	34.185	5
3N/O	2.07(2)	2(2)					
1N/O	2.19(2)	2(2)	neg2(3)	0.0561	176.709	36.838	5
4N/O	2.07(2)	4(2)					
1N/O	2.20(3)	1(3)	neg2(2)	0.0507	159.832	33.320	5
3N/O	2.05(2)	3(2)					
2N/O	2.18(3)	2(3)	neg3(2)	0.0497	156.751	32.678	5
5N/O	2.09(3)	7(3)					
1N/O	2.20(0.10)	4(10)	neg2(3)	0.0572	180.192	37.564	5
4N/O	2.07(5)	7(5)					
2N/O	2.17(0.10)	6(11)	neg3(3)	0.0581	183.108	38.172	5
3N/O	2.08(9)	7(6)					
3N/O	2.13(0.13)	10(13)	neg3(3)	0.0591	186.472	38.874	5
6N/O	2.11(6)	12(4)					
1N/O	2.09(7)	4(7)	neg3(3)	0.0650	204.927	42.721	5
5N/O	2.11(2)	7(2)					
2N/O	2.28(0.31)	33(62)	neg1(5)	0.0574	180.906	37.713	5
4N/O	2.10(2)	6(2)					
3N/O	2.15(0.25)	25(16)	neg2(6)	0.0615	193.786	40.398	5

Co-S(2.2) Co-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(4)	4(3)					
1S	2.30(6)	2(4)	neg21(8)	0.1432	451.497	94.123	5
2S	2.16(5)	5(4)					
2S	2.29(7)	7(6)	neg20(7)	0.1179	371.831	77.515	5
3S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.19(4)	8(4)					
2S	2.33(9)	10(9)	neg18(7)	0.1050	331.152	69.035	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.21(4)	9(3)					
2S	2.38(9)	12(10)	neg17(6)	0.0957	301.577	62.869	5
3S	2.33(9)	15(12)					
3S	2.20(4)	9(4)	neg18(7)	0.1009	318.132	66.321	5
6S	2.23(4)	13(2)					
1S	2.46(7)	8(8)	neg18(5)	0.0934	294.435	61.381	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.21(3)	10(3)					
3S	2.39(7)	16(10)	neg16(5)	0.0870	274.210	57.164	5

Co-N(2.0) Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(4)	2(2)					5
1S	2.29(5)	4(3)	neg9(7)	0.1326	418.037	87.148	
1N/O	2.00(5)	1(3)					5
2S	2.25(4)	6(3)	neg15(7)	0.1428	450.325	93.879	
2N/O	2.04(4)	3(3)					
2S	2.28(5)	9(4)	neg11(7)	0.1167	368.046	76.726	5
3N/O	2.06(3)	4(2)	neg6(5)	0.0988	311.467	64.931	5

1S	2.32(5)	7(5)					
1N/O 3S			No Fit	No Fit	No Fit	No Fit	5
1N/O 4S			No Fit	No Fit	No Fit	No Fit	5
4N/O 1S	2.10(2) 2.51(0.28)	5(1) 29(42)	neg1(4)	0.0793	249.878	52.092	5
2N/O 3S			No Fit	No Fit	No Fit	No Fit	5
3N/O 2S	2.07(3) 2.31(7)	5(2) 13(6)	neg7(5)	0.0978	308.437	64.300	5
5N/O 1S			No Fit	No Fit	No Fit	No Fit	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.10(2) 2.54(0.19)	5(1) 35(29)	neg1(3)	0.0722	227.652	47.458	5
2N/O 4S			No Fit	No Fit	No Fit	No Fit	5
3N/O 3S	2.07(3) 2.31(8)	5(2) 19(7)	neg8(6)	0.0964	303.898	63.353	5
6N/O 1S			No Fit	No Fit	No Fit	No Fit	5
1N/O 6S			No Fit	No Fit	No Fit	No Fit	5
5N/O 2S	2.11(2) 2.64(9)	7(1) 28(16)	neg1(2)	0.0503	158.544	33.051	5
2N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 3S	2.10(2) 2.55(0.17)	5(1) 39(24)	neg1(3)	0.0677	213.390	44.485	5
3N/O 4S			No Fit	No Fit	No Fit	No Fit	5

Table F.4. Additional Fits for Co(II) E34A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	2(1)	1(5)	0.3083	883.830	52.616	3
3N/O	2.11(2)	4(1)	-1(3)	0.1940	643.435	38.305	3
4N/O	2.11(1)	5(1)	-1(2)	0.1329	440.929	26.249	3
5N/O	2.11(1)	7(1)	-1(2)	0.1055	350.133	20.844	3
6N/O	2.11(1)	9(1)	-2(2)	0.0998	331.148	19.714	3
7N/O	2.10(1)	10(1)	-3(2)	0.1078	357.529	21.284	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.20(3)	6(1)	-21(6)	0.2762	916.139	54.539	3
3S	2.20(2)	8(1)	-21(4)	0.2028	672.701	40.047	3
4S	2.21(2)	11(1)	-22(4)	0.1690	560.643	33.376	3
5S	2.21(2)	12(1)	-22(4)	0.1554	515.519	30.690	3
6S	2.21(2)	14(1)	-22(3)	0.1527	506.519	30.154	3
7S	2.21(2)	16(1)	-22(3)	0.1560	517.511	30.808	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.05(1)	1(1)					
1N/O	2.18(1)	4(1)	-2(2)	0.1161	385.280	26.036	5
2N/O	2.03(1)	1(1)					
2N/O	2.17(1)	1(1)	-3(2)	0.0867	287.478	19.427	5
3N/O	2.06(1)	2(1)					
1N/O	2.19(2)	3(1)	-2(2)	0.0911	302.139	20.418	5
4N/O	2.07(1)	4(1)					
1N/O	2.20(2)	1(2)	-3(2)	0.0890	295.253	19.952	5
3N/O	2.05(2)	3(1)					
2N/O	2.18(2)	1(2)	-3(2)	0.0879	291.440	19.695	5
5N/O	2.08(2)	7(2)					
1N/O	2.19(4)	2(4)	-3(2)	0.0981	325.406	21.990	5
4N/O	2.06(3)	6(3)					
2N/O	2.17(4)	4(4)	-3(2)	0.0993	329.523	22.268	5

3N/O	2.05(4)	6(4)					
3N/O	2.16(3)	6(5)	-3(2)	0.1010	335.193	22.651	5
6N/O	2.11(5)	12(3)					
1N/O	2.10(7)	4(6)	-3(2)	0.1082	358.920	24.255	5
5N/O	2.11(2)	7(1)					
2N/O	2.28(0.25)	34(49)	-1(4)	0.1003	332.871	22.495	5
4N/O	2.12(0.10)	17(7)					
3N/O	2.10(2)	6(2)	-3(3)	0.1089	361.102	24.402	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.16(3)	4(2)					
1S	2.29(4)	2(2)	-21(5)	0.1801	597.399	40.371	5
2S	2.16(3)	6(3)					
2S	2.29(5)	7(4)	-20(5)	0.1569	520.636	35.183	5
3S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.19(3)	8(3)					
2S	2.33(7)	11(7)	-18(5)	0.1443	478.850	32.359	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.21(2)	10(2)					
2S	2.38(6)	13(7)	-17(4)	0.1346	446.506	30.174	5
3S	2.33(7)	15(9)					
3S	2.20(3)	9(3)	-18(5)	0.1402	464.967	31.421	5
6S	2.23(2)	13(1)					
1S	2.46(5)	8(5)	-17(3)	0.1314	436.008	29.464	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.22(2)	10(2)					
3S	2.39(5)	16(7)	-16(4)	0.1261	418.342	28.270	5

Co-N(2.0) Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(3)	2(2)					5
1S	2.29(3)	3(2)	-10(4)	0.1691	560.979	37.910	
1N/O	1.99(3)	1(2)					5
2S	2.25(3)	6(2)	-15(5)	0.1764	585.197	39.546	
2N/O	2.03(3)	4(2)					
2S	2.28(3)	9(2)	-11(4)	0.1547	513.056	34.671	5
3N/O	2.06(2)	4(1)					
1S	2.31(3)	6(3)	-7(4)	0.1391	461.388	31.179	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(2)	5(1)					
1S	2.55(0.19)	29(31)	-1(3)	0.1201	398.413	26.924	5
2N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.06(3)	5(2)					
2S	2.31(4)	13(4)	-8(4)	0.1383	458.646	30.994	5
5N/O							
1S			No Fit	No Fit	No Fit	No Fit	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(1)	5(1)					
2S	2.56(0.13)	34(21)	-1(2)	0.1125	373.266	25.224	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.07						
3S	2.31(5)	18(5)	-8(4)	0.1372	455.114	30.755	5
6N/O	2.11(1)	9(1)					
1S	1.98(0.13)	33(42)	-1(2)	0.0991	328.776	22.218	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.12(1)	7(1)	1(2)	0.0892	295.960	20.000	5

2S	2.66(6)	25(10)					
2N/O	1.79(6)	15(10)					
5S	2.19(2)	12(1)	-25(4)	0.1413	468.593	31.666	5
4N/O	2.11(1)	5(1)					
3S	2.57(0.11)	38(17)	-1(2)	0.1076	356.906	24.119	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Co-N(2.0) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.12(2)	7(2)					
1Imd	2.02(4)	5(4)	-3(2)	0.0796	263.910	17.834	5
4N/O	2.11(1)	5(1)					
1Imd	2.18(3)	3(3)					
1Imd	2.00(2)	2(2)	-2(1)	0.0579	191.984	15.001	7
3N/O	2.11(1)	3(1)					
1Imd	2.00(3)	0(2)					
1Imd	2.27(0.10)	8(17)					
1Imd	2.16(4)	0(5)	-1(2)	0.0522	173.202	16.040	9
2N/O	2.10(1)	1(2)					
1Imd	1.89(4)	1(6)					
1Imd	1.99(3)	9(4)					
1Imd	2.12(3)	10(4)					
1Imd	2.24(3)	7(3)	-3(2)	0.0545	180.720	20.541	11
1N/O	2.10(2)	3(2)					
1Imd	2.24(6)	15(6)					
1Imd	2.13(5)	17(6)					
1Imd	2.35(8)	7(10)					
1Imd	2.01(5)	15(6)					
1Imd	1.92(5)	8(6)	-1(3)	0.0708	234.824	34.544	13
4N/O	2.12(1)	5(1)					
1Imd	2.01(3)	3(2)	-2(2)	0.0878	291.265	19.683	5
3N/O	2.11(1)	3(1)					
1Imd	2.00(2)	0(1)					
1Imd	2.18(3)	1(2)	-2(1)	0.0577	191.260	14.945	7
2N/O	2.11(1)	1(1)					
1Imd	2.24(5)	0(8)					
1Imd	2.13(5)	2(7)					
1Imd	1.99(3)	2(3)	-1(2)	0.0635	210.774	19.520	9

1N/O							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1Imd	1.92(8)	6(16)					
1Imd	2.11(0.17)	13(20)					
1Imd	2.00(9)	13(16)					
1Imd	2.21(0.34)	10(36)					
1Imd	2.26(0.50)	3(89)	-2(3)	0.2116	702.106	79.804	11
3N/O	2.12(2)	3(1)					
1Imd	2.01(3)	1(2)	-2(2)	0.1206	400.225	27.046	5
2N/O	2.10(2)	1(1)					
1Imd	2.18(2)	1(2)					
1Imd	2.01(2)	1(1)	-2(2)	0.0820	272.163	21.266	7
1N/O	2.10(2)	2(2)					
1Imd	1.99(3)	5(2)					
1Imd	2.24(3)	5(3)					
1Imd	2.11(3)	6(3)	-1(2)	0.1025	339.894	31.478	9
0N/O							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O	2.13(2)	1(2)					
1Imd	2.02(3)	1(2)	-2(3)	0.1939	643.173	43.464	5
1N/O	2.10(2)	2(2)					
1Imd	2.18(2)	3(2)					
1Imd	2.02(2)	2(1)	-1(3)	0.1492	494.791	38.662	7
0N/O							
1Imd	2.12(4)	8(4)					
1Imd	2.00(3)	6(3)					
1Imd	2.23(4)	5(5)	-1(3)	0.2624	870.328	68.006	7

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	3(2)					
1S	2.34(5)	11(6)					
1Imd	1.98(3)	2(2)	-5(3)	0.0938	311.236	24.319	7

2N/O	2.10(1)	1(1)					
1S	2.48(0.10)	22(15)					
1Imd	2.17(2)	1(2)					
1Imd	2.01(2)	1(1)	-2(2)	0.0634	210.272	19.474	9
1N/O	2.10(2)	2(2)					
1S	2.49(0.14)	23(24)					
1Imd	1.98(4)	4(3)					
1Imd	2.10(5)	6(5)					
1Imd	2.22(4)	4(5)	-1(3)	0.0835	276.911	31.475	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	3(2)					
1S	2.35(5)	12(7)					
1Imd	1.98(3)	2(2)	-5(3)	0.0955	316.747	24.750	7
2N/O	2.10(1)	1(1)					
1S	2.50(0.10)	24(16)					
1Imd	2.01(2)	1(1)					
1Imd	2.18(2)	1(2)	-2(2)	0.0630	208.903	19.347	9
1N/O	2.10(2)	2(2)					
1S	2.52(0.14)	24(23)					
1Imd	2.10(4)	6(4)					
1Imd	1.98(3)	4(3)					
1Imd	2.23(4)	5(4)	-1(3)	0.0826	274.102	31.156	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	3(1)					
1S	2.36(5)	13(7)					
1Imd	1.98(3)	2(2)	-5(3)	0.0968	321.237	25.101	7
2N/O	2.10(1)	1(1)					
1S	2.52(0.10)	24(16)					
1Imd	2.18(2)	1(2)					
1Imd	2.01(2)	1(1)	-2(2)	0.0623	206.716	19.144	9
1N/O	2.10(2)	2(2)					
1S	2.54(0.14)	23(21)					
1Imd	1.98(3)	5(3)					
1Imd	2.23(4)	5(4)					
1Imd	2.10(4)	6(4)	-1(2)	0.0817	270.879	30.789	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	3(1)					
1S	2.36(6)	14(8)					
1Imd	1.98(3)	2(2)	-5(3)	0.0978	324.435	25.351	7
2N/O	2.10(1)	1(1)					
1S	2.53(0.10)	25(16)					
1Imd	2.01(2)	1(1)					
1Imd	2.18(2)	1(2)	-2(2)	0.0616	204.312	18.922	9
1N/O	2.10(2)	2(2)					
1S	2.55(0.13)	23(20)					
1Imd	2.23(3)	5(4)					
1Imd	1.98(3)	5(3)					
1Imd	2.11(4)	6(4)	-1(2)	0.0807	267.564	30.412	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	3(1)					
1S	2.37(6)	15(9)					
1Imd	1.98(3)	2(2)	-5(3)	0.0986	326.951	25.547	7
2N/O	2.10(1)	1(1)					
1S	2.54(0.10)	25(16)					
1Imd	2.01(2)	1(1)					
1Imd	2.18(2)	1(2)	-2(2)	0.0609	202.055	18.713	9
1N/O	2.10(2)	2(2)					
1S	2.57(0.12)	22(18)					
1Imd	1.98(3)	5(3)					
1Imd	2.23(3)	5(3)					
1Imd	2.11(4)	7(3)	-1(2)	0.0797	264.283	30.040	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	4(2)					
1Br	2.47(7)	18(9)					
1Imd	2.02(4)	2(3)	-2(3)	0.1174	389.400	30.427	7
2N/O	2.08(3)	1(2)					
1Br	2.13(6)	15(9)					
1Imd	1.99(3)	1(2)					
1Imd	2.16(3)	1(2)	-3(2)	0.0781	259.220	24.007	9
1N/O	2.11(2)	2(2)					
1Br	2.43(5)	14(7)					
1Imd	2.27(4)	5(4)	1(2)	0.0930	308.659	35.083	11

1Imd	2.14(4)	7(3)					
1Imd	2.01(3)	5(2)					

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(2)	5(3)					
1Br	2.47(6)	17(7)					
1Imd	2.08(8)	7(9)	-1(3)	0.1170	388.007	30.318	7
2N/O	2.10(2)	1(2)					
1Br	2.25(0.33)	36(53)					
1Imd	2.18(3)	1(2)					
1Imd	2.01(2)	1(2)	-2(2)	0.0798	264.804	24.524	9
1N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(2)	5(3)					
1Br	2.47(6)	17(7)					
1Imd	2.09(8)	8(9)	-1(3)	0.1158	384.006	30.006	7
2N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Co-N(2.0) Co-S(2.2) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	4(2)					
1Br	2.47(7)	18(8)					
1Imd	2.03(4)	3(3)	-2(3)	0.1152	382.136	29.859	7
2N/O	2.10(2)	1(2)					
1Br	2.36(0.26)	34(41)					
1Imd	2.01(2)	1(2)	-2(2)	0.0790	261.935	24.258	9

1Imd	2.18(3)	1(2)					

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	3(2)					
1S	2.26(3)	5(2)					
1Br	2.20(4)	1(3)					
1Imd	1.93(5)	5(5)	-10(3)	0.0876	290.664	26.919	9
1N/O	2.09(2)	3(2)					
1S	2.42(6)	1(5)					
1Br	2.39(6)	3(5)					
1Imd	2.15(2)	2(2)					
1Imd	1.99(2)	3(2)	-3(2)	0.0543	180.218	20.484	11
1N/O	1.99(5)	4(3)					
1S	2.23(6)	1(3)					
2Br	2.12(6)	11(10)					
1Imd	1.93(5)	3(4)	-13(5)	0.1295	429.596	39.785	9
0N/O							
1S	2.22(5)	4(4)	-14(6)	0.2191	726.961	56.803	7

1N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

3Br	2.03(5)	18(7)
1Imd	1.95(5)	2(4)

Co-N(2.0) Co-S(2.2) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	3(2)					
1S	2.26(3)	4(2)					
1Br	2.20(4)	1(3)					
1Imd	1.93(5)	4(5)	-10(3)	0.0860	285.363	26.428	9
1N/O	2.09(2)	3(2)					
1S	2.42(5)	1(5)					
1Br	2.39(6)	5(5)					
1Imd	1.99(2)	3(1)					
1Imd	2.15(2)	3(2)	-3(2)	0.0521	172.996	19.663	11
0N/O							
1S	2.39(0.10)	7(14)					
1Br	2.39(9)	9(7)					
1Imd	2.25(6)	4(7)					
1Imd	2.13(4)	7(4)					
1Imd	2.00(3)	6(3)	-1(3)	0.1591	527.921	60.006	11
1N/O	1.44(4)	7(5)					
1S	2.32(8)	9(8)					
2Br	2.00(4)	11(3)					
1Imd	1.94(5)	2(4)	-11(7)	0.1618	536.622	49.697	9

Co-N(2.0) Co-S(2.4) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(4)	1(3)					
1S	2.33(7)	1(5)					
1Br	2.29(0.11)	7(8)					
1Imd	1.96(5)	1(3)	-7(4)	0.0970	321.952	29.816	9
1N/O	2.09(2)	3(2)					
1S	2.44(6)	3(6)					
1Br	2.40(6)	1(5)					
1Imd	1.99(2)	3(1)					
1Imd	2.15(2)	2(2)	-3(2)	0.0520	172.407	19.596	11
0N/O							
1S	2.44(2)	12(3)					
1Br	2.39(2)	7(3)					
1Imd	2.01(3)	8(2)					
1Imd	2.18(3)	6(2)	-3(2)	0.1063	352.669	40.086	11

1Imd	2.04(0.14)	8(21)					
1N/O	2.00(6)	4(3)					
1S	2.24(6)	1(3)					
2Br	2.11(7)	13(13)					
1Imd	1.92(5)	2(4)	-14(5)	0.1377	456.787	42.303	9

Co-N(2.0) Co-S(2.4) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	3(2)					
1S	2.27(4)	4(3)					
1Br	2.21(4)	1(4)					
1Imd	1.92(5)	3(4)	-11(4)	0.0914	303.289	28.088	9
1N/O	2.09(2)	3(1)					
1S	2.44(5)	1(5)					
1Br	2.40(5)	3(5)					
1Imd	2.15(2)	2(2)					
1Imd	1.99(2)	3(1)	-3(2)	0.0503	166.851	18.965	11
0N/O							
1S	2.41(9)	5(14)					
1Br	2.39(8)	8(8)					
1Imd	2.00(3)	6(3)					
1Imd	2.12(4)	7(5)					
1Imd	2.24(6)	3(8)	-2(3)	0.1607	533.152	60.600	11
1N/O	1.98(5)	5(3)					
1S	2.22(6)	2(4)					
2Br	2.11(6)	10(9)					
1Imd	1.92(5)	3(5)	-15(5)	0.1295	429.577	39.784	9

Co-N(2.0) Co-S(2.6) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(2)	1(2)					
1S	2.42(0.10)	2(9)					
1Br	2.39(0.10)	5(7)					
1Imd	1.98(4)	1(2)	-5(4)	0.0938	311.042	28.806	9
1N/O	2.08(2)	3(2)					
1S	2.47(4)	6(4)					
1Br	2.42(4)	2(3)					
1Imd	2.00(2)	3(1)					
1Imd	2.16(3)	2(2)	-3(2)	0.0470	155.782	17.707	11
0N/O							
1S	2.44(2)	11(2)					
1Br	2.38(2)	7(2)	-4(2)	0.0933	309.576	35.188	11

1Imd	2.02(3)	8(2)					
1Imd	1.97(6)	2(10)					
1Imd	2.17(2)	8(2)					
1N/O	2.10(5)	4(4)					
1S	2.37(0.11)	2(8)					
2Br	2.35(0.13)	12(9)					
1Imd	1.99(5)	1(3)	-6(6)	0.1683	558.180	51.694	9

Co-N(2.0) Co-S(2.6) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(2)	1(2)					
1S	2.40(9)	3(8)					
1Br	2.38(0.10)	7(6)					
1Imd	1.98(4)	1(2)	-6(4)	0.0930	308.429	28.564	9
1N/O	2.09(1)	3(1)					
1S	2.46(5)	2(5)					
1Br	2.42(5)	2(4)					
1Imd	2.15(2)	2(1)					
1Imd	1.99(2)	3(1)	-3(2)	0.0478	158.497	18.015	11
0N/O							
1S	2.45(3)	11(3)					
1Br	2.40(3)	6(3)					
1Imd	2.04(4)	8(3)					
1Imd	2.19(2)	8(3)					
1Imd	1.98(5)	2(9)	-3(2)	0.1180	391.562	44.507	11
1N/O	2.05(2)	3(2)					
1S	2.54(2)	5(1)					
2Br	2.49(2)	3(1)					
1Imd	2.13(4)	1(4)	-1(2)	0.1184	392.681	36.367	9

Co-N(2.2) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(2)	5(1)					
1S	2.61(0.10)	23(18)					
1Imd	2.01(3)	3(2)	-3(2)	0.0722	239.468	18.712	7
3N/O	2.11(1)	4(1)					
1S	2.60(7)	19(10)					
1Imd	2.01(2)	0(1)					
1Imd	2.18(3)	1(2)	-2(1)	0.0462	153.216	14.190	9
2N/O	2.12(1)	2(2)					
1S	2.65(5)	12(6)					
1Imd	2.14(3)	5(3)	1(2)	0.0488	161.920	18.404	11

1Imd	2.27(4)	3(3)					
1Imd	2.01(3)	4(2)					
1N/O	2.1(2)	3(2)					
1S	2.46(0.14)	20(21)					
1Imd	2.23(4)	9(3)					
1Imd	2.11(4)	12(3)					
1Imd	1.99(4)	11(4)					
1Imd	1.89(5)	4(6)	-4(3)	0.067	222.200	32.687	13
0N/O							
1S	2.29(4)	5(5)					
1Imd	1.91(8)	6(14)					
1Imd	2.32(0.10)	10(13)					
1Imd	2.22(0.10)	15(13)					
1Imd	2.00(9)	14(12)					
1Imd	2.11(0.10)	16(13)	-3(5)	0.1581	524.326	77.131	13

Co-N(2.2) Co-Br(2.3) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.13(2)	6(2)					
1Br	2.40(8)	22(13)					
1Imd	2.01(3)	3(2)	-3(2)	0.2263	750.701	110.432	7
3N/O	2.12(2)	4(1)					
1Br	2.34(0.11)	24(16)					
1Imd	2.18(3)	1(3)					
1Imd	2.01(2)	0(1)	-3(1)	0.0786	260.838	38.371	9
2N/O	2.12(2)	2(2)					
1Br	2.42(6)	16(7)					
1Imd	2.15(3)	5(3)					
1Imd	2.01(3)	4(2)					
1Imd	2.28(4)	3(4)	-1(2)	0.0543	180.103	20.471	11
1N/O	2.11(3)	1(2)					
1Br	2.43(7)	13(7)					
1Imd	2.18(0.12)	7(14)					
1Imd	2.30(8)	5(11)					
1Imd	2.01(0.49)	0(60)					
1Imd	2.06(0.41)	4(29)	-1(4)	0.052	172.636	15.988	13
0N/O							
1Br							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Co-N(2.2) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(2)	6(2)					
1Br	2.40(8)	22(12)					
1Imd	2.02(3)	3(2)	-3(2)	0.0717	238.001	18.597	7
3N/O	2.12(2)	4(1)					
1Br	2.35(0.10)	24(15)					
1Imd	2.18(3)	1(2)					
1Imd	2.01(2)	0(1)	-3(1)	0.0513	170.222	15.764	9
2N/O	2.12(2)	2(2)					
1Br	2.42(6)	16(7)					
1Imd	2.01(3)	4(2)					
1Imd	2.28(4)	3(4)					
1Imd	2.15(3)	5(3)	-1(2)	0.0528	175.249	19.920	11
1N/O	2.11(3)	1(3)					
1Br	2.43(7)	13(7)					
1Imd	2.01(0.46)	0(58)					
1Imd	2.18(0.11)	7(14)					
1Imd	2.30(8)	5(11)					
1Imd	2.06(0.38)	4(27)	-1(3)	0.0771	255.681	37.612	13
0N/O							
1Br							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Co-N(2.2) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(2)	6(2)					
1Br	2.41(7)	21(11)					
1Imd	2.02(7)	21(11)	-3(2)	0.1729	573.488	84.363	7
3N/O	2.12(1)	4(1)					
1Br	2.37(9)	23(13)					
1Imd	2.18(3)	1(2)					
1Imd	2.01(2)	0(1)	-3(1)	0.0744	246.856	36.314	9
2N/O	2.12(2)	2(2)					
1Br	2.43(5)	16(6)					
1Imd	2.28(4)	2(4)					
1Imd	2.01(3)	4(2)	-1(2)	0.0504	167.278	19.013	11

1Imd	2.15(3)	5(3)					
1N/O	2.11(3)	1(3)					
1Br	2.44(6)	13(7)					
1Imd	2.06(0.35)	4(24)					
1Imd	2.18(0.11)	7(13)					
1Imd	2.01(0.44)	0(56)					
1Imd	2.30(8)	5(11)	-1(3)	0.05	165.796	15.355	13
0N/O							
1Br							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Co-N(2.2) Co-Br(2.7) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	7(2)					
1Br	2.87(3)	12(4)					
1Imd	2.08(6)	7(8)	-3(2)	0.0626	207.807	16.238	7
3N/O	2.11(1)	5(2)					
1Br	2.86(3)	12(4)					
1Imd	2.18(2)	0(2)					
1Imd	2.02(2)	0(2)	-3(1)	0.0405	134.237	12.432	9
2N/O	2.11(2)	3(2)					
1Br	2.85(4)	12(4)					
1Imd	2.26(5)	1(6)					
1Imd	2.15(3)	4(4)					
1Imd	2.01(3)	3(2)	-1(2)	0.043	142.526	16.200	11
1N/O	2.11(3)	1(3)					
1Br	2.83(5)	12(6)					
1Imd	2.25(3)	8(5)					
1Imd	2.13(3)	10(5)					
1Imd	2.01(4)	9(6)					
1Imd	1.93(7)	0(11)	-2(2)	0.0638	211.538	31.118	13

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.12(2)	5(1)					
1S	2.50(0.22)	33(31)					
1Imd	2.01(3)	3(3)	-3(2)	0.0804	266.692	20.839	7
3N/O	2.11(1)	3(1)	-1(1)	0.0451	149.605	13.855	9

1S	2.60(7)	21(12)					
1Imd	2.01(2)	0(1)					
1Imd	2.19(2)	0(2)					
2N/O	2.11(1)	1(1)					
1S	2.65(5)	13(7)					
1Imd	2.14(3)	5(3)					
1Imd	2.01(3)	4(2)					
1Imd	2.27(4)	3(3)	-1(2)	0.049	162.697	18.493	11
1N/O	2.09(2)	3(2)					
1S	2.47(0.14)	21(21)					
1Imd	2.23(4)	9(3)					
1Imd	1.99(4)	11(4)					
1Imd	2.11(4)	12(3)					
1Imd	1.89(5)	3(6)	-4(3)	0.0676	224.264	32.990	13
0N/O							
1S	2.29(5)	5(5)					
1Imd	1.91(9)	6(14)					
1Imd	2.10(0.10)	16(13)					
1Imd	2.21(011)	15(13)					
1Imd	2.32(0.10)	10(13)					
1Imd	2.00(9)	14(12)	-3(5)	0.1664	552.013	81.204	13

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	7(2)					
1S	2.68(5)	16(8)					
1Imd	2.12(8)	9(10)	-1(2)	0.0758	251.491	19.651	7
3N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O	2.11(1)	1(1)					
1S	2.66(5)	14(7)					
1Imd	2.27(4)	3(3)					
1Imd	2.01(3)	3(2)					
1Imd	2.14(3)	5(3)	-1(2)	0.0453	150.217	17.074	11
1N/O	2.10(2)	3(2)					
1S	2.51(0.13)	22(19)					
1Imd	2.23(3)	9(3)					
1Imd	1.90(5)	3(6)					
1Imd	1.99(3)	11(4)	-3(2)	0.0651	215.995	31.774	13

1Imd	2.11(3)	12(3)					

Co-N(2.0) Co-S(2.7) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	7(2)					
1S	2.68(5)	15(8)					
1Imd	2.12(8)	9(10)	-1(2)	0.0747	247.876	19.369	7
3N/O	2.11(1)	3(1)					
1S	2.63(6)	20(10)					
1Imd	2.01(2)	1(1)					
1Imd	2.19(2)	0(2)	-1(1)	0.0411	136.363	12.629	9
2N/O	2.11(1)	1(1)					
1S	2.66(5)	14(7)					
1Imd	2.27(4)	3(3)					
1Imd	2.01(3)	3(2)					
1Imd	2.14(3)	5(3)	1(2)	0.0445	147.625	16.780	11
1N/O							
1S							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Co-N(2.0) Co-S(2.2) Co-Br(2.7) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	2(1)					
1Br	2.92(2)	9(2)					
1S	2.57(7)	18(11)					
1Imd	2.20(2)	1(2)	1(2)	0.0666	220.969	20.464	9
2N/O	2.09(2)	2(2)					
1Br	2.86(3)	11(4)					
1S	2.47(7)	17(8)					
1Imd	2.02(3)	1(2)					
1Imd	2.18(2)	2(1)	-2(2)	0.0389	129.019	14.665	11
1N/O	2.10(3)	1(3)					
1Br	2.84(5)	11(5)					
1S	2.44(9)	17(15)					
1Imd	2.11(0.35)	1(51)					
1Imd	2.19(0.43)	0(41)					
1Imd	1.99(9)	2(10)	-2(3)	0.0574	190.566	28.033	13

Co-N(2.0) Co-S(2.3) Co-Br(2.7) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	2(1)					
1Br	2.92(2)	9(2)					
1S	2.58(7)	18(10)					
1Imd	2.20(2)	1(1)	1(2)	0.0653	216.680	20.067	9
2N/O	2.09(2)	1(2)					
1Br	2.86(3)	11(4)					
1S	2.48(7)	18(9)					
1Imd	2.02(3)	1(2)					
1Imd	2.18(2)	2(1)	-2(2)	0.0387	128.439	14.599	11
1N/O							
1Br							
1S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Co-N(2.0) Co-S(2.6) Co-Br(2.7) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	3(2)					
1Br	2.41(7)	9(6)					
1S	2.44(8)	6(9)					
1Imd	2.00(4)	3(3)	-4(3)	0.0683	226.527	20.979	9
2N/O	2.09(1)	1(1)					
1Br	2.46(4)	5(4)					
1S	2.50(4)	2(5)					
1Imd	2.00(2)	1(1)					
1Imd	2.16(2)	1(1)	-2(1)	0.293	97.091	11.036	11
1N/O	2.09(1)	3(1)					
1Br	2.43(5)	2(8)					
1S	2.47(5)	2(8)					
1Imd	1.99(2)	4(2)					
1Imd	2.13(3)	4(4)					
1Imd	2.24(6)	2(11)	-2(2)	0.0357	118.366	17.412	13

Co-N(2.0) Co-S(2.7) Co-Br(2.7) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(1)	1(1)					
1Br	2.47(4)	4(4)					
1S	2.51(4)	1(5)					
1Imd	2.16(2)	1(1)					
1Imd	2.00(2)	1(1)	-2(1)	0.0283	93.823	10.664	11

Co-N(2.0) Co-N(2.2) Co-S(2.7) Co-Br(2.7) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(1)	5(1)					
1N/O	2.16(1)	6(1)					
1Br	2.50(3)	3(3)					
1S	2.54(4)	1(4)					
1Imd	2.02(7)	6(9)					
1Imd	2.16(8)	6(11)	-2(2)	0.017	56.437	8.302	13

Co-N(2.0) Co-N(2.2) Co-S(2.7) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(1)	5(1)					
1N/O	2.16(1)	6(1)					
1Br	2.50(3)	2(4)					
1S	2.54(4)	1(4)					
1Imd	2.02(7)	6(10)					
1Imd	2.16(8)	6(11)	-2(2)	0.0174	57.746	8.495	13

Co-N(2.0) Co-N(2.2) Co-S(2.6) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(1)	5(1)					
1N/O	2.16(1)	6(1)					
1Br	2.54(4)	3(4)					
1S	2.49(4)	1(4)					
1Imd	2.02(8)	6(10)					
1Imd	2.16(8)	6(12)	-2(2)	0.0183	60.850	8.951	13

Co-N(2.0) Co-N(2.2) Co-S(2.6) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(3)	8(2)					
1N/O	2.16(2)	9(2)					
1Br	2.23(5)	1(3)					
1S	2.43(5)	4(3)					
1Imd	1.98(7)	4(7)					
1Imd	2.14(4)	0(3)	-2(2)	0.0239	79.172	11.647	13

Co-N(2.0) Co-N(2.2) Co-S(2.6) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(3)	8(2)					
1N/O	2.16(3)	10(2)					
1Br	2.23(5)	1(3)					
1S	2.42(5)	4(3)					
1Imd	2.01(5)	0(4)					
1Imd	2.16(6)	1(5)	-2(2)	0.0246	81.489	11.987	13

Table F.5. Additional Fits for Zn(II) E34A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

	Zn-N(2.0)						
N	**Radius Å**	**σ^2 (x10^{-3} $Å^2$)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.14(5)	3(4)	12(8)	0.4724	6944.925	1021.782	3
3N/O	2.12(4)	5(4)	9(6)	0.3984	5855.812	861.545	3
4N/O	2.11(4)	7(3)	7(5)	0.3727	5478.543	806.039	3
5N/O	2.10(4)	9(4)	5(5)	0.3755	5520.384	812.194	3
6N/O	2.09(5)	10(4)	3(5)	0.3952	5808.758	854.622	3
7N/O	2.08(5)	12(4)	2(5)	0.4238	6230.333	916.647	3

	Zn-S(2.2)						
N	**Radius Å**	**σ^2 (x10^{-3} $Å^2$)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.27(3)	5(2)	neg2(6)	0.2518	3701.262	544.554	3
3S	2.25(3)	8(2)	neg5(5)	0.1978	2907.231	427.731	3
4S	2.24(3)	10(2)	neg7(5)	0.1854	2726.047	401.074	3
5S	2.24(3)	12(2)	neg9(5)	0.1951	2868.536	422.038	3
6S	2.23(4)	14(2)	neg10(5)	0.2163	3180.225	467.895	3
7S	2.22(4)	16(2)	neg11(5)	0.2431	3573.563	525.766	3

	Zn-N(2.0) Zn-N(2.2)						
	r(Å)	**σ^2(x10^{-3} $Å^2$)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.05(3)	2(2)					
1N/O	2.19(3)	6(2)	6(4)	0.2065	3035.794	632.869	5
2N/O	2.02(3)	2(2)					
2N/O	2.17(3)	3(2)	5(4)	0.2310	3395.115	707.777	5
3N/O	2.05(3)	1(3)					
1N/O	2.19(3)	5(2)	5(4)	0.2144	3151.071	656.901	5
4N/O	2.05(3)	4(3)					
1N/O	2.19(3)	4(2)	3(4)	0.2507	3685.128	768.235	5
3N/O	2.02(3)	1(3)					
2N/O	2.17(3)	2(2)	3(4)	0.2743	4031.516	840.446	5
5N/O	2.05(4)	6(4)					
1N/O	2.18(3)	3(3)	2(5)	0.3005	4416.638	920.732	5
4N/O	2.02(4)	4(4)					
2N/O	2.17(4)	1(3)	2(5)	0.3290	4836.271	1008.213	5
3N/O	2.00(4)	2(4)					
3N/O	2.15(4)	1(3)	1(5)	0.3527	5184.583	1080.825	5

6N/O	2.04(5)	8(4)					
1N/O	2.18(4)	3(3)	1(5)	0.3542	5206.067	1085.304	5
5N/O	2.02(5)	7(5)					
2N/O	2.16(5)	0(4)	0(5)	0.3846	5653.323	1178.543	5
4N/O	2.00(6)	6(6)					
3N/O	2.15(5)	2(5)	0(6)	0.4091	6013.678	1253.666	5

Zn-S(2.2) Zn-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.16(2)	3(1)					
1S	2.30(2)	2(1)	ne11(4)	0.0657	965.276	201.230	5
2S	2.13(2)	3(2)					
2S	2.28(2)	1(1)	neg12(4)	0.0820	1204.945	251.194	5
3S	2.16(2)	6(2)					
1S	2.30(2)	1(1)	neg12(4)	0.0759	1116.196	232.692	5
4S	2.26(4)	11(3)					
1S	1.81(0.10)	22(19)	neg2(7)	0.1666	2449.314	510.606	5
3S	2.14(3)	7(2)					
2S	2.28(3)	2(2)	neg13(4)	0.1149	1688.698	352.041	5
5S	2.25(5)	13(3)					
1S	1.84(0.17)	26(35)	neg6(8)	0.1828	2686.953	560.147	5
4S	2.25(3)	6(2)					
2S	2.09(4)	5(3)	neg13(5)	0.1537	2259.033	470.939	5
3S	2.11(4)	8(3)					
3S	2.27(3)	5(2)	neg14(5)	0.1634	2402.459	500.838	5
6S	2.23(5)	14(4)					
1S	1.88(0.21)	22(28)	neg8(9)	0.1970	2895.560	603.635	5
5S	2.25(5)	13(3)					
2S	1.85(0.12)	34(31)	neg4(9)	0.1760	2586.594	539.225	5
4S	2.25(4)	7(3)					
3S	2.10(5)	9(5)	neg14(6)	0.1924	2828.919	589.742	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(2)	1(2)					5
1S	2.30(2)	0(1)	0(3)	0.0691	1015.782	211.759	

1N/O 2S	1.98(2) 2.27(2)	2(2) 4(1)	neg4(3)	0.0724	1063.735	221.756	5
2N/O 2S	1.99(3) 2.28(2)	3(2) 4(2)	neg3(4)	0.1049	1541.868	321.426	5
3N/O 1S	2.03(3) 2.30(2)	4(2) 1(1)	0(4)	0.0916	1346.236	280.649	5
1N/O 3S	1.96(3) 2.26(2)	1(2) 7(2)	neg6(4)	0.1118	1642.774	342.467	5
1N/O 4S	2.13(0.42) 2.25(4)	18(204) 11(7)	neg6(12)	0.1792	2634.626	549.238	5
4N/O 1S	2.03(4) 2.30(3)	7(3) 1(2)	0(5)	0.1294	1901.497	396.403	5
2N/O 3S	2.07(0.17) 2.27(5)	14(29) 9(5)	neg2(10)	0.1663	2444.686	509.641	5
3N/O 2S	2.01(6) 2.28(3)	8(4) 5(2)	neg3(6)	0.1483	2179.348	454.327	5
5N/O 1S	2.04(7) 2.29(3)	11(5) 2(3)	0(6)	0.1667	2450.822	510.921	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.13(0.18) 2.28(4)	17(24) 7(5)	3(14)	0.1568	2305.173	480.557	5
2N/O 4S	2.16(0.35) 2.25(0.35)	20(171) 11(7)	neg4(17)	0.1729	2541.409	529.805	5
3N/O 3S	2.14(0.12) 2.27(4)	17(60) 9(7)	1(15)	0.1600	2352.500	490.423	5
6N/O 1S	2.06(0.11) 2.29(3)	16(6) 3(3)	0(8)	0.1956	2876.000	599.557	5
1N/O 6S	2.19(3) 2.20(3)	3(2) 11(2)	neg12(4)	0.1148	1688.042	351.905	5
5N/O 2S	2.17(0.17) 2.29(4)	22(28) 6(3)	5(14)	0.1572	2310.904	481.752	5
2N/O	2.20(2)	2(1)	neg10(4)	0.0706	1038.447	216.484	5

5S	2.21(2)	8(1)					
4N/O	2.19(8)	18(51)					
3S	2.28(3)	9(4)	3(14)	0.1507	2214.641	461.684	5
3N/O	2.18(0.31)	19(154)					
4S	2.26(4)	11(9)	neg2(24)	0.1655	2432.936	507.192	5

Zn-N(2.0) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.04(4)	3(2)					5
1Br	2.42(3)	4(1)	neg1(7)	0.1184	1740.113	362.760	
1N/O	1.37(0.12)	7(13)					5
2Br	2.35(6)	8(2)	neg19(17)	0.3428	5039.320	1050.542	
2N/O	2.01(3)	3(2)					
2Br	2.40(3)	8(1)	neg6(6)	0.0826	1214.449	253.175	5
3N/O	2.05(3)	5(2)					
1Br	2.43(2)	5(1)	0(4)	0.0720	1058.900	220.756	5
1N/O	1.95(3)	0(2)					
3Br	2.36(3)	10(1)	neg16(7)	0.1067	1568.003	326.880	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.05(3)	7(2)					
1Br	2.43(2)	5(1)	0(4)	0.0602	885.144	184.525	5
2N/O	1.99(3)	3(2)					
3Br	2.39(3)	10(1)	neg10(6)	0.0699	1027.418	214.185	5
3N/O	2.03(3)	6(2)					
2Br	2.42(2)	8(1)	neg3(4)	0.0514	756.113	157.626	5
5N/O	2.05(3)	9(2)					
1Br	2.42(2)	5(1)	neg1(4)	0.0682	1001.922	208.870	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.04(3)	8(2)					
2Br	2.42(2)	8(1)	neg3(3)	0.0436	640.301	133.483	5
2N/O	1.97(3)	4(2)					
4Br	2.39(3)	12(1)	neg12(6)	0.0678	997.191	207.884	5

3N/O	2.01(3)	6(2)					
3Br	2.41(2)	10(1)	neg5(4)	0.0502	737.747	153.797	5
6N/O	2.05(3)	11(2)					
1Br	2.42(2)	5(1)	neg2(4)	0.0862	1267.491	264.233	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.04(3)	10(2)					
2Br	2.42(2)	9(1)	neg3(4)	0.0502	737.378	153.721	5
2N/O	1.96(4)	4(2)					
5Br	2.38(3)	13(1)	neg13(6)	0.0712	1046.902	218.247	5
4N/O	2.03(3)	9(2)					
3Br	2.42(2)	11(1)	neg4(4)	0.0450	661.054	137.809	5
3N/O	2.00(3)	7(2)					
4Br	2.41(2)	12(1)	neg7(5)	0.0560	823.404	171.654	5

Table F.6. Additional Fits for Zn(II) E34A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.14(2)	3(3)	11(0)	0.5132	8230.214	489.956	3
3N/O	2.12(3)	5(2)	9(4)	0.4437	7115.043	423.569	3
4N/O	2.11(3)	7(2)	7(4)	0.4189	6717.437	399.899	3
5N/O	2.10(3)	9(3)	5(4)	0.4212	6753.882	402.068	3
6N/O	2.09(3)	10(3)	3(4)	0.4394	7046.090	419.464	3
7N/O	2.08(3)	12(3)	2(4)	0.4662	7475.706	445.039	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.27(2)	6(1)	-2(5)	0.3101	4972.113	295.997	3
3S	2.25(2)	8(1)	-5(4)	0.2589	4150.898	247.109	3
4S	2.24(2)	10(1)	-7(4)	0.2468	3957.136	235.574	3
5S	2.24(2)	12(2)	-9(4)	0.2554	4095.326	243.801	3
6S	2.23(3)	14(2)	-10(4)	0.2749	4407.425	262.380	3
7S	2.22(3)	16(2)	-11(4)	0.2996	4803.779	285.976	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar

2N/O	2.05(2)	1(2)					
1N/O	2.19(2)	5(1)	6(3)	0.2835	4546.172	307.218	5
2N/O	2.02(2)	1(2)					
2N/O	2.17(2)	2(1)	5(3)	0.3028	4856.279	328.175	5
3N/O	2.05(2)	1(2)					
1N/O	2.19(2)	5(1)	5(3)	0.2858	4582.443	309.669	5
4N/O	2.05(2)	4(2)					
1N/O	2.19(2)	4(2)	3(3)	0.3158	5063.945	342.208	5
3N/O	2.02(2)	2(2)					
2N/O	2.17(2)	2(2)	3(3)	0.3374	5411.009	365.662	5
5N/O	2.05(3)	6(2)					
1N/O	2.18(2)	3(2)	2(3)	0.3593	5761.536	389.349	5
4N/O	2.02(3)	4(2)					
2N/O	2.17(2)	1(2)	2(3)	0.3847	6169.295	416.905	5
3N/O	2.00(3)	2(3)					
3N/O	2.15(3)	1(2)	2(3)	0.4070	6526.952	441.074	5
6N/O	2.04(3)	8(3)					
1N/O	2.18(3)	2(2)	1(3)	0.4073	6531.207	441.362	5
5N/O	2.02(3)	7(3)					
2N/O	2.16(3)	0(3)	0(3)	0.4343	6964.237	470.625	5
4N/O	2.00(4)	6(4)					
3N/O	2.15(3)	2(3)	0(4)	0.4568	7325.268	495.022	5

Zn-S(2.2) Zn-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.17(2)	3(1)					
1S	2.30(2)	1(1)	-1(3)	0.1373	2201.927	148.800	5
2S	2.13(2)	3(1)					
2S	2.28(2)	2(1)	-11(3)	0.1513	2425.435	163.905	5
3S	2.17(2)	6(1)					
1S	2.30(2)	0(1)	-12(3)	0.1455	2333.795	157.712	5
4S	2.26(3)	11(2)					
1S	1.81(7)	22(14)	-3(5)	0.2299	3686.402	249.117	5
3S	2.14(2)	7(2)					
2S	2.28(2)	3(1)	-13(3)	0.1809	2900.152	195.985	5

5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.25(2)	6(1)					
2S	2.09(3)	5(2)	-13(3)	0.2180	3496.326	236.273	5
3S	2.12(3)	8(2)					
3S	2.27(2)	5(2)	-14(4)	0.2257	3620.020	244.631	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.25(3)	13(2)					
2S	1.85(9)	24(22)	-5(6)	0.2382	3819.479	258.110	5
4S	2.26(3)	7(2)					
3S	2.10(4)	9(3)	-14(4)	0.2540	4073.059	275.247	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(2)	1(1)					5
1S	2.30(2)	0(1)	0(3)	0.1419	2275.606	153.780	
1N/O	1.98(2)	1(1)					5
2S	2.27(2)	4(1)	-3(3)	0.1462	2345.128	158.478	
2N/O	1.99(2)	3(2)					
2S	2.28(2)	4(1)	-3(3)	0.1723	2762.598	186.689	5
3N/O	2.03(2)	4(2)					
1S	2.30(2)	1(1)	0(3)	0.1607	2576.731	174.129	5
1N/O	1.96(2)	0(2)					
3S	2.26(2)	7(1)	-5(3)	0.1801	2888.186	195.176	5
1N/O	2.12(0.27)	18(130)					
4S	2.25(3)	11(5)	-6(8)	0.2411	3866.573	261.293	5
4N/O	2.03(3)	7(2)					
1S	2.30(2)	1(1)	0(3)	0.1950	3127.073	211.319	5
2N/O	2.06(0.12)	13(6)					
3S	2.26(3)	9(3)	-3(6)	0.2296	3681.096	248.759	5
3N/O	2.01(4)	7(3)					
2S	2.28(2)	5(2)	-3(4)	0.2116	3393.662	229.335	5
5N/O	2.04(4)	11(3)	0(4)	0.2300	3687.886	249.218	5

1S	2.30(2)	2(2)					
1N/O	2.45(2)	3(1)					
5S	2.20(3)	14(2)	-14(4)	0.1476	2367.248	159.972	5
4N/O	2.12(0.12)	17(15)					
2S	2.28(3)	7(3)	2(9)	0.2235	3584.467	242.229	5
2N/O	2.16(0.24)	22(119)					
4S	2.25(3)	11(4)	-4(12)	0.2356	3778.779	255.360	5
3N/O	2.13(9)	18(37)					
3S	2.27(3)	9(4)	0(10)	0.2256	3618.025	244.497	5
6N/O	2.06(7)	16(4)					
1S	2.29(2)	3(2)	0(6)	0.2577	4132.860	279.288	5
1N/O	2.19(2)	3(1)					
6S	2.21(2)	11(1)	-11(3)	0.1862	2985.227	201.734	5
5N/O	2.16(0.12)	22(19)					
2S	2.29(3)	6(2)	4(10)	0.2252	3611.869	244.081	5
2N/O	2.20(2)	2(1)					
5S	2.21(2)	8(1)	-9(3)	0.1459	2340.192	158.144	5
4N/O	2.17(7)	20(38)					
3S	2.28(3)	9(3)	2(11)	0.2193	3516.995	237.669	5
3N/O	2.18(0.19)	22(102)					
4S	2.26(3)	11(4)	-3(16)	0.2296	3682.206	248.834	5

Zn-N(2.0) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.04(3)	2(2)					5
1Br	2.42(2)	4(1)	-2(5)	0.1782	2857.194	193.082	
1N/O	1.37(7)	8(8)					5
2Br	2.35(4)	8(2)	-18(10)	0.3910	6270.363	423.735	
2N/O	2.01(3)	3(2)					
2Br	2.40(2)	8(1)	-6(5)	0.1453	2330.338	157.478	5
3N/O	2.05(2)	5(1)					
1Br	2.42(2)	5(1)	-1(3)	0.1359	2178.544	147.220	5
1N/O	1.96(3)	0(2)					
3Br	2.37(2)	10(1)	-16(5)	0.1723	2762.179	186.661	5

1N/O	1.95(2)	0(2)					
4Br	2.36(2)	11(1)	-17(5)	0.1568	2514.998	169.957	5
4N/O	2.05(2)	7(2)					
1Br	2.42(1)	5(1)	-1(3)	0.1252	2007.797	135.682	5
2N/O	1.99(3)	3(2)					
3Br	2.40(2)	10(1)	-9(5)	0.1346	2158.227	145.847	5
3N/O	2.02(2)	6(2)					
2Br	2.42(2)	8(1)	-4(4)	0.1172	1879.056	126.982	5
5N/O	2.05(2)	9(2)					
1Br	2.42(1)	5(1)	-1(3)	0.1328	2129.939	143.936	5
1N/O	2.68(3)	4(2)					
5Br	2.24(4)	14(1)	-42(9)	0.2344	3759.139	254.033	5
4N/O	2.03(2)	8(2)					
2Br	2.42(2)	8(1)	-3(3)	0.1107	1775.572	119.989	5
2N/O	1.98(3)	4(2)					
4Br	2.39(2)	12(1)	-11(5)	0.1337	2143.854	144.876	5
3N/O	2.01(3)	6(2)					
3Br	2.41(2)	10(1)	-6(4)	0.1165	1867.592	126.207	5
6N/O	2.05(3)	11(2)					
1Br	2.42(1)	5(1)	-2(3)	0.1498	2401.949	162.317	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.04(3)	10(2)					
2Br	2.42(2)	9(1)	-3(3)	0.1173	1880.882	127.105	5
2N/O	1.97(3)	4(2)					
5Br	2.38(2)	13(1)	-13(5)	0.1377	2207.405	149.171	5
4N/O	2.02(3)	9(2)					
3Br	2.42(2)	11(1)	-4(4)	0.1126	1805.039	121.980	5
3N/O	2.00(3)	7(2)					
4Br	2.41(2)	12(1)	-7(4)	0.1222	1959.681	132.430	5

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	3(2)					
1S	2.26(5)	3(2)	-5(5)	0.0846	1356.190	105.970	7

1Br	2.42(2)	7(3)					
1N/O	1.97(3)	1(3)					
2S	2.23(7)	8(2)					
1Br	2.40(2)	6(3)	-8(6)	0.0878	1408.371	110.047	7
1N/O	1.97(3)	1(2)					
1S	2.25(4)	3(3)					
2Br	2.42(3)	11(3)	-6(5)	0.0891	1428.039	111.584	7
3N/O	2.02(4)	7(3)					
1S	2.25(7)	7(5)					
1Br	2.42(2)	6(2)	-4(5)	0.0912	1461.919	114.232	7
2N/O	2.01(4)	6(4)					
2S	2.23(8)	12(5)					
1Br	2.41(2)	5(1)	-7(6)	0.0894	1434.243	112.069	7
2N/O	2.00(3)	3(2)					
1S	2.28(4)	4(3)					
2Br	2.41(2)	11(3)	-4(4)	0.0822	1317.680	102.961	7

Zn-N(2.0) Zn-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.06(4)	10(4)					
1Imd	2.16(5)	1(4)	3(4)	0.3742	5624.547	380.092	5
4N/O	2.04(5)	12(7)					
1Imd	2.17(3)	4(2)					
1Imd	2.04(4)	3(3)	2(3)	0.2920	4682.365	365.871	7
3N/O	1.98(8)	20(15)					
1Imd	1.95(3)	9(2)					
1Imd	2.07(3)	12(2)					
1Imd	2.19(2)	11(2)	0(3)	0.2268	3636.635	336.792	9
2N/O	2.06(7)	8(10)					
1Imd	1.85(5)	6(6)					
1Imd	1.95(4)	13(4)					
1Imd	2.07(3)	15(3)					
1Imd	2.19(3)	13(2)	-2(3)	0.2041	3272.665	371.985	11
1N/O	2.08(6)	0(7)					
1Imd	1.84(5)	13(9)					
1Imd	1.95(4)	18(6)					
1Imd	1.71(0.12)	5(25)					
1Imd	2.18(4)	16(4)					
1Imd	2.06(4)	19(5)	-3(4)	0.1598	2563.084	377.043	13

4N/O	2.06(3)	7(3)					
1Imd	2.18(4)	0(3)	5(3)	0.3577	5736.406	387.651	5
3N/O	2.04(5)	9(7)					
1Imd	2.04(4)	2(3)					
1Imd	2.18(3)	4(2)	2(3)	0.2829	4535.757	354.416	7
2N/O	1.99(8)	14(16)					
1Imd	2.20(3)	10(2)					
1Imd	1.96(3)	8(3)					
1Imd	2.07(3)	12(2)	1(3)	0.2250	3608.253	334.164	9
1N/O	2.07(7)	2(8)					
1Imd	2.07(3)	16(3)					
1Imd	1.96(3)	15(3)					
1Imd	1.85(3)	9(4)					
1Imd	2.19(2)	14(2)	-2(3)	0.1868	2995.615	340.494	11
0N/O							
1Imd	1.73(0.24)	19(45)					
1Imd	1.86(4)	11(5)					
1Imd	2.19(3)	15(3)					
1Imd	2.08(3)	18(3)					
1Imd	1.96(3)	17(4)	-2(4)	0.1872	3001.804	341.197	11
3N/O	2.06(3)	5(3)					
1Imd	2.18(3)	1(3)	6(4)	0.3614	5795.490	391.644	5
2N/O	2.04(6)	6(7)					
1Imd	2.04(4)	2(4)					
1Imd	2.18(3)	4(2)	3(3)	0.2898	4645.917	363.101	7
1N/O	2.04(9)	5(11)					
1Imd	2.07(3)	11(2)					
1Imd	1.95(3)	8(3)					
1Imd	2.19(2)	10(2)	1(3)	0.2292	3675.286	340.372	9
0N/O							
1Imd	1.87(3)	10(3)					
1Imd	1.97(2)	16(2)					
1Imd	2.20(2)	15(2)					
1Imd	2.08(2)	17(2)	-2(2)	0.1978	3171.666	293.731	9
2N/O	2.06(4)	2(3)					
1Imd	2.18(3)	2(3)	7(4)	0.4010	6430.608	434.564	5
1N/O	2.04(8)	3(9)					
1Imd	2.17(3)	4(2)					
1Imd	2.04(4)	3(3)	4(4)	0.3272	5247.070	409.996	7

0N/O							
1Imd	2.19(2)	11(2)					
1Imd	2.06(2)	12(2)					
1Imd	1.95(2)	9(2)	1(2)	0.2622	4204.364	328.521	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	3(2)					
1S	2.30(1)	0(1)					
1Imd	2.07(3)	1(3)	0(2)	0.0994	1493.700	116.715	7
1N/O	1.99(2)	1(2)					
1S	2.30(1)	0(1)					
1Imd	2.17(0.22)	19(56)					
1Imd	2.08(3)	0(3)	1(4)	0.0771	1236.623	114.525	9
0N/O							
1S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	3(2)					
1S	2.30(1)	1(1)					
1Imd	2.07(3)	1(3)	-1(2)	0.0969	1554.363	121.455	7
1N/O	1.99(2)	3(2)					
1S	2.29(1)	0(1)					
1Imd	1.92(4)	1(3)					
1Imd	2.08(3)	2(2)	-3(2)	0.0677	1085.818	100.559	9
0N/O							
1S	2.28(2)	2(2)					
1Imd	2.20(3)	6(3)					
1Imd	2.07(3)	8(2)					
1Imd	1.94(2)	6(2)	0(2)	0.0888	1424.699	131.943	11

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	4(3)					
1S	2.30(1)	1(1)					
1Imd	2.07(4)	2(3)	-1(2)	0.0961	1541.701	120.466	7
1N/O	1.99(2)	1(2)					
1S	2.30(1)	1(1)	-1(3)	0.0727	1165.405	107.929	9

1Imd	2.08(4)	1(3)					
1Imd	2.13(0.21)	15(37)					
0N/O							
1S	2.28(2)	2(2)					
1Imd	2.20(3)	6(3)					
1Imd	1.95(2)	6(2)					
1Imd	2.07(3)	8(2)	0(2)	0.0854	1369.528	126.833	11

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(3)	2(3)					
1S	2.72(5)	6(5)					
1Imd	2.17(3)	1(3)	5(4)	0.3338	5353.170	418.287	7
1N/O	2.01(9)	5(13)					
1S	2.67(3)	1(2)					
1Imd	2.01(4)	4(2)					
1Imd	2.14(3)	5(2)	0(3)	0.2116	3393.344	314.261	9
0N/O							
1S	2.67(3)	2(3)					
1Imd	1.94(2)	8(2)					
1Imd	2.18(2)	10(2)					
1Imd	2.06(2)	11(2)	-1(2)	0.1978	3171.671	293.732	11

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(3)	2(3)					
1S	2.72(5)	6(6)					
1Imd	2.17(3)	2(3)	5(4)	0.3375	5411.380	422.835	7
1N/O	2.00(9)	5(12)					
1S	2.67(3)	1(2)					
1Imd	2.01(4)	4(2)					
1Imd	2.14(3)	5(2)	0(3)	0.2173	3484.187	322.674	9
0N/O							
1S	2.67(3)	3(3)					
1Imd	1.94(2)	8(2)					
1Imd	2.18(2)	10(2)					
1Imd	2.06(2)	11(2)	-1(2)	0.2033	3259.561	301.871	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.43(2)	8(2)	-3(2)	0.0323	517.513	47.927	9

1Imd	2.06(2)	1(2)					
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.43(2)	8(2)					
1Imd	2.06(2)	1(2)	-2(2)	0.0315	504.914	46.761	9
0N/O							
1S	2.25(3)	8(3)					
1Br	2.42(1)	5(1)					
1Imd	2.09(2)	2(2)					
1Imd	1.96(1)	2(1)	-4(2)	0.0291	467.250	43.272	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.43(2)	8(2)					
1Imd	2.06(2)	1(2)	-2(2)	0.0309	495.371	45.877	9
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.44(2)	8(2)					
1Imd	2.06(2)	1(2)	-2(2)	0.0304	487.566	45.154	9
0N/O							
1S	2.26(3)	7(3)					
1Br	2.43(1)	6(1)					
1Imd	2.09(2)	2(2)					
1Imd	1.96(1)	2(1)	-4(2)	0.0303	486.069	45.015	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(2)					
1Br	2.43(2)	8(2)					
1Imd	2.06(3)	1(2)	-3(2)	0.0335	536.436	49.680	9
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.43(2)	8(2)					
1Imd	2.06(2)	1(2)	-3(2)	0.0326	522.802	48.417	9
0N/O							
1S	2.26(3)	8(3)					
1Br	2.42(1)	5(1)					
1Imd	1.96(1)	2(1)					
1Imd	2.09(2)	2(2)	-4(2)	0.0289	463.561	42.931	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.43(2)	8(2)					
1Imd	2.06(2)	1(2)	-3(2)	0.0319	512.207	47.436	9
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.43(2)	8(2)	-3(2)	0.0314	503.492	46.629	9

1Imd	2.06(2)	1(2)					
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(2)					
1Br	2.42(2)	8(2)					
1Imd	2.06(3)	1(2)	-3(2)	0.0348	558.349	51.709	9
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(2)					
1Br	2.43(2)	8(2)					
1Imd	2.06(3)	1(2)	-3(2)	0.0339	544.151	50.394	9
0N/O							
1S	2.27(3)	8(3)					
1Br	2.42(1)	5(1)					
1Imd	2.09(2)	3(2)					
1Imd	1.96(1)	2(1)	-4(2)	0.0289	463.351	42.911	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(2)					
1Br	2.43(2)	8(2)					
1Imd	2.06(2)	1(2)	-3(2)	0.0332	532.991	49.361	9
0N/O							
1S	2.27(3)	8(3)					
1Br	2.42(1)	6(1)					
1Imd	1.96(1)	2(1)					
1Imd	2.09(2)	2(2)	-4(2)	0.0293	469.445	43.476	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(1)					
1Br	2.43(2)	8(2)					
1Imd	2.06(2)	1(2)	-3(2)	0.0327	523.789	48.509	9
0N/O							
1S	2.27(3)	8(3)					
1Br	2.42(1)	6(1)					
1Imd	2.09(2)	2(2)					
1Imd	1.96(1)	2(1)	-4(2)	0.0296	474.665	43.959	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(3)	3(2)					
1Br	2.42(2)	8(2)					
1Imd	2.06(3)	1(2)	-3(3)	0.0360	578.057	53.534	9
0N/O							
1S	2.27(3)	9(3)					
1Br	2.42(1)	5(1)					
1Imd	1.96(1)	2(1)					
1Imd	2.09(2)	3(2)	-4(2)	0.0289	463.807	42.954	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(2)					
1Br	2.42(2)	8(2)					
1Imd	2.06(3)	1(2)	-3(2)	0.0351	563.324	52.170	9
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	0(2)					
1S	2.28(2)	3(2)					
1Br	2.43(2)	8(2)	-3(2)	0.0344	551.712	51.095	9

1Imd	2.06(3)	1(2)					
0N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	2(2)					
1S	2.78(4)	2(3)					
1Br	2.42(2)	4(1)					
1Imd	2.10(3)	2(2)	0(4)	0.1101	1765.503	163.505	9
0N/O							
1S	2.92(7)	13(11)					
1Br	2.43(1)	4(1)					
1Imd	2.10(2)	5(1)					
1Imd	1.97(2)	5(1)	-2(2)	0.0759	1217.889	112.790	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	1(3)					
1S	2.78(4)	3(3)					
1Br	2.41(2)	4(1)					
1Imd	2.10(3)	1(2)	0(4)	0.1096	1757.434	162.758	9
0N/O							
1S	2.94(7)	13(10)					
1Br	2.42(1)	4(1)					
1Imd	1.97(2)	5(1)					
1Imd	2.10(2)	5(1)	-2(2)	0.0711	1140.917	105.661	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	1(2)					
1S	2.78(4)	3(3)					
1Br	2.42(2)	4(1)					
1Imd	2.10(3)	1(2)	0(4)	0.1108	1776.991	164.569	9
0N/O							
1S	2.94(7)	13(10)					
1Br	2.43(1)	4(1)					
1Imd	1.97(2)	5(1)					
1Imd	2.10(2)	5(1)	-2(2)	0.0728	1167.898	108.160	9

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.01(5)	11(5)					
1S	2.30(2)	1(1)					
1Imd	2.04(3)	1(2)	-2(3)	0.1276	1918.340	149.895	7
2N/O	1.99(4)	6(4)					
1S	2.28(2)	2(1)					
1Imd	2.50(3)	1(3)					
1Imd	2.04(4)	2(3)	-4(3)	0.0791	1268.494	117.477	9
1N/O	1.98(2)	2(3)					
1S	2.28(2)	0(2)					
1Imd	1.90(5)	2(4)					
1Imd	2.06(3)	1(2)					
1Imd	2.50(4)	2(4)	-6(3)	0.0533	854.925	97.174	11

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.01(5)	12(5)					
1S	2.30(2)	1(1)					
1Imd	2.04(3)	1(2)	-2(3)	0.1236	1981.261	154.812	7
2N/O	2.01(3)	3(2)					
1S	2.31(2)	0(1)					
1Imd	2.39(0.18)	14(24)					
1Imd	2.09(4)	1(3)	1(3)	0.0879	1410.000	130.582	9
1N/O	1.98(2)	2(3)					
1S	2.28(2)	0(2)					
1Imd	1.90(5)	2(4)					
1Imd	2.49(4)	2(5)					
1Imd	2.06(3)	1(2)	-6(3)	0.0525	842.548	95.767	11

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.01(6)	13(6)					
1S	2.30(2)	1(1)					
1Imd	2.03(2)	1(2)	-2(3)	0.1214	1946.630	152.106	7
2N/O	2.01(3)	3(2)					
1S	2.31(2)	0(1)					
1Imd	2.09(4)	1(3)					
1Imd	2.35(0.20)	16(30)	1(3)	0.0877	1405.862	130.198	9
1N/O	1.98(2)	2(3)					
1S	2.28(2)	1(2)	-6(3)	0.0531	851.274	96.759	11

1Imd	2.49(4)	2(5)					
1Imd	2.06(3)	1(2)					
1Imd	1.90(5)	3(4)					

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(3)	5(3)					
1S	2.70(4)	5(4)					
1Imd	2.17(3)	1(3)	4(3)	0.2824	4528.648	353.860	7
2N/O	2.00(3)	2(2)					
1S	2.28(3)	1(2)					
1Imd	2.51(4)	1(4)					
1Imd	1.40(0.13)	24(22)	-4(4)	0.1049	1682.104	155.781	9
1N/O	1.95(0.10)	8(18)					
1S	2.67(3)	2(3)					
1Imd	2.07(3)	11(3)					
1Imd	1.95(3)	8(3)					
1Imd	2.19(3)	10(2)	-1(2)	0.1560	2501.925	284.379	11

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(3)	5(3)					
1S	2.71(4)	6(5)					
1Imd	2.17(3)	1(3)	4(3)	0.2867	4597.499	359.240	7
2N/O	2.01(5)	8(8)					
1S	2.67(2)	2(2)					
1Imd	2.02(3)	4(2)					
1Imd	2.15(3)	5(2)	0(3)	0.1775	2845.877	263.560	9
1N/O	1.95(0.10)	8(18)					
1S	2.67(3)	3(3)					
1Imd	2.19(3)	10(2)					
1Imd	2.07(3)	11(3)					
1Imd	1.96(3)	8(3)	-1(2)	0.1606	2575.681	292.762	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	8(4)					
1S	2.27(4)	6(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	3(2)	-4(3)	0.0414	663.691	61.465	9
1N/O	1.99(5)	8(7)					
1S	2.26(3)	10(4)	-3(2)	0.0191	306.820	34.874	11

1Br	2.42(1)	5(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.11(2)	2(2)					
0N/O							
1S	2.24(2)	7(3)					
1Br	2.42(1)	5(1)					
1Imd	1.96(2)	3(2)					
1Imd	1.86(6)	10(10)					
1Imd	2.09(2)	4(2)	-6(2)	0.0213	341.912	38.863	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	8(4)					
1S	2.28(4)	6(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	2(2)	-4(3)	0.0414	663.513	61.449	9
1N/O	1.98(5)	8(7)					
1S	2.27(3)	10(4)					
1Br	2.43(1)	6(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.11(2)	2(2)	-3(2)	0.0193	310.204	35.259	11
0N/O							
1S	2.24(2)	7(3)					
1Br	2.42(1)	5(1)					
1Imd	2.09(2)	4(2)					
1Imd	1.86(6)	10(10)					
1Imd	1.96(2)	3(2)	-6(2)	0.0217	348.516	39.614	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	8(4)					
1S	2.28(3)	5(3)					
1Br	2.42(1)	7(1)					
1Imd	2.04(3)	2(2)	-4(3)	0.0415	665.216	61.606	9
1N/O	1.98(5)	8(7)					
1S	2.27(3)	9(4)					
1Br	2.43(1)	6(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.11(2)	2(2)	-3(2)	0.0197	315.770	35.892	11
0N/O							
1S	2.25(2)	7(3)					
1Br	2.42(1)	5(1)					
1Imd	2.09(2)	4(2)	-6(2)	0.0224	359.176	40.825	11

1Imd	1.86(7)	11(11)					
1Imd	1.96(2)	3(2)					

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(4)					
1S	2.28(3)	5(2)					
1Br	2.42(1)	7(1)					
1Imd	2.04(3)	2(2)	-4(3)	0.0415	665.795	61.660	9
1N/O	1.97(4)	8(6)					
1S	2.27(3)	9(4)					
1Br	2.43(1)	6(1)					
1Imd	2.11(2)	2(2)					
1Imd	1.98(2)	1(2)	-3(2)	0.0200	320.927	36.478	11
0N/O							
1S	2.25(2)	7(3)					
1Br	2.42(1)	5(1)					
1Imd	2.09(2)	4(2)					
1Imd	1.96(2)	3(2)					
1Imd	1.87(7)	11(11)	-6(2)	0.0230	369.044	41.947	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	9(4)					
1S	2.28(4)	7(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	3(2)	-4(3)	0.0412	660.267	61.148	9
1N/O	1.99(5)	8(6)					
1S	2.27(3)	11(4)					
1Br	2.42(1)	5(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.11(2)	2(2)	-3(1)	0.0187	299.938	34.092	11
0N/O							
1S	2.25(3)	8(3)					
1Br	2.42(1)	5(1)					
1Imd	2.09(2)	4(2)					
1Imd	1.96(2)	3(2)					
1Imd	1.87(7)	11(11)	-6(2)	0.0213	340.877	38.745	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	8(4)	-4(3)	0.0411	659.155	61.045	9

1S	2.28(4)	6(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	2(2)					
1N/O	1.98(5)	8(6)					
1S	2.27(3)	10(4)					
1Br	2.42(1)	6(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.11(2)	2(2)	-3(1)	0.0188	301.945	34.320	11
0N/O							
1S	2.26(2)	8(3)					
1Br	2.43(1)	6(1)					
1Imd	2.19(3)	2(4)					
1Imd	1.95(2)	4(2)					
1Imd	2.07(2)	6(3)	-1(1)	0.0225	360.969	41.029	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	8(4)					
1S	2.28(3)	6(3)					
1Br	2.42(1)	7(1)					
1Imd	2.04(3)	2(2)	-4(3)	0.0412	659.999	61.123	9
1N/O	1.98(5)	8(6)					
1S	2.28(3)	10(4)					
1Br	2.43(1)	6(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.11(2)	2(2)	-3(1)	0.0191	306.164	34.800	11
0N/O							
1S	2.25(3)	8(3)					
1Br	2.42(1)	5(1)					
1Imd	1.96(2)	3(2)					
1Imd	2.09(2)	3(2)					
1Imd	1.87(7)	11(12)	-6(2)	0.0220	353.405	40.169	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	7(6)					
1S	2.28(3)	5(3)					
1Br	2.42(1)	7(1)					
1Imd	2.04(3)	2(2)	-3(1)	0.0411	659.846	61.109	9
1N/O	1.98(4)	7(6)					
1S	2.28(3)	9(4)					
1Br	2.43(1)	6(1)					
1Imd	2.11(2)	2(2)	-3(1)	0.0193	310.138	35.252	11

1Imd	1.98(2)	1(2)					
0N/O							
1S	2.26(2)	8(3)					
1Br	2.43(1)	6(1)					
1Imd	1.95(2)	4(2)					
1Imd	2.07(2)	6(3)					
1Imd	2.19(3)	3(4)	-1(1)	0.0236	378.924	43.070	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	9(4)					
1S	2.28(4)	7(3)					
1Br	2.41(1)	6(1)					
1Imd	2.04(3)	3(2)	-4(3)	0.0413	662.701	61.373	9
1N/O	1.99(5)	8(6)					
1S	2.27(3)	11(5)					
1Br	2.42(1)	5(1)					
1Imd	2.11(2)	2(2)					
1Imd	1.98(2)	1(2)	-3(1)	0.0185	297.246	33.786	11
0N/O							
1S	2.25(3)	8(3)					
1Br	2.42(1)	5(1)					
1Imd	1.96(2)	3(2)					
1Imd	1.88(7)	11(12)					
1Imd	2.09(2)	3(2)	-6(2)	0.0213	342.174	38.893	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	9(4)					
1S	2.28(4)	6(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	3(2)	-4(3)	0.0412	661.282	61.242	9
1N/O	1.99(5)	8(6)					
1S	2.28(3)	11(4)					
1Br	2.42(1)	6(1)					
1Imd	2.11(2)	2(2)					
1Imd	1.98(2)	1(2)	-3(1)	0.0186	298.486	33.927	11
0N/O							
1S	2.25(3)	8(3)					
1Br	2.42(1)	5(1)					
1Imd	2.09(2)	3(2)					
1Imd	1.96(2)	3(2)					
1Imd	1.88(7)	11(12)	-6(2)	0.0215	344.398	39.146	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	8(4)					
1S	2.28(4)	6(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	2(2)	-4(3)	0.0413	661.856	61.295	9
1N/O	1.98(5)	8(6)					
1S	2.28(3)	10(4)					
1Br	2.43(1)	6(1)					
1Imd	2.11(2)	2(2)					
1Imd	1.98(2)	1(2)	-3(1)	0.0188	301.976	34.324	11
0N/O							
1S	2.26(2)	9(3)					
1Br	2.43(1)	6(1)					
1Imd	2.07(2)	6(3)					
1Imd	2.19(3)	3(4)					
1Imd	1.95(2)	4(2)	-1(1)	0.0226	362.727	41.229	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	8(4)					
1S	2.28(3)	6(3)					
1Br	2.42(1)	7(1)					
1Imd	2.04(3)	2(2)	-4(3)	0.0413	661.489	61.261	9
1N/O	1.98(4)	7(6)					
1S	2.28(3)	10(4)					
1Br	2.43(1)	6(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.11(2)	2(2)	-3(1)	0.0190	305.339	34.706	11
0N/O							
1S	2.26(2)	8(3)					
1Br	2.43(1)	6(1)					
1Imd	2.19(3)	3(4)					
1Imd	1.95(2)	4(2)					
1Imd	2.07(2)	6(3)	-1(1)	0.0230	369.329	41.979	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	9(4)					
1S	2.28(4)	7(3)					
1Br	2.41(1)	6(1)	-4(3)	0.0414	664.665	61.555	9

1Imd	2.04(3)	3(2)					
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.26(3)	9(4)					
1Br	2.42(1)	6(1)					
1Imd	2.19(3)	3(4)					
1Imd	2.07(2)	6(3)					
1Imd	1.95(2)	4(2)	-1(1)	0.0214	342.743	38.958	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	9(4)					
1S	2.28(4)	7(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	3(2)	-4(3)	0.0413	662.647	61.368	9
1N/O	1.99(5)	8(6)					
1S	2.28(3)	11(4)					
1Br	2.42(1)	6(1)					
1Imd	2.11(2)	2(2)					
1Imd	1.98(2)	1(2)	-3(1)	0.0185	296.765	33.732	11
0N/O							
1S	2.26(2)	9(4)					
1Br	2.42(1)	6(1)					
1Imd	1.95(2)	4(2)					
1Imd	2.19(3)	3(4)					
1Imd	2.07(2)	6(3)	-1(1)	0.0219	350.784	39.872	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	9(4)					
1S	2.28(4)	6(3)					
1Br	2.42(1)	6(1)					
1Imd	2.04(3)	2(2)	-4(3)	0.0413	662.737	61.377	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

0N/O							
1S	2.27(2)	9(3)					
1Br	2.42(1)	6(1)					
1Imd	2.19(3)	3(4)					
1Imd	2.07(2)	6(3)					
1Imd	1.95(2)	4(2)	-1(1)	0.0223	357.270	40.609	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(2)	3(2)					
1S	2.80(3)	4(3)					
1Br	2.43(1)	4(1)					
1Imd	2.11(3)	0(2)	0(3)	0.0664	1064.478	98.582	9
1N/O	2.03(4)	4(5)					
1S	2.89(7)	14(11)					
1Br	2.43(1)	4(1)					
1Imd	1.98(2)	3(2)					
1Imd	2.11(2)	4(1)	-1(2)	0.0379	608.103	69.119	11
0N/O							
1S	2.93(7)	13(10)					
1Br	2.43(1)	4(1)					
1Imd	2.11(4)	4(3)					
1Imd	1.98(0.18)	7(24)					
1Imd	1.98(6)	4(3)	-3(3)	0.0547	877.246	99.711	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(2)	3(2)					
1S	2.79(3)	6(3)					
1Br	2.42(1)	4(1)					
1Imd	2.11(4)	1(2)	0(3)	0.0657	1052.774	97.498	9
1N/O	2.02(4)	4(5)					
1S	2.92(8)	18(14)					
1Br	2.43(1)	4(1)					
1Imd	1.98(2)	3(2)					
1Imd	2.11(2)	4(1)	-1(2)	0.0337	540.468	61.432	11
0N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Table F.7. Additional Fits for Ni(II) E34C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	1(2)	7(4)	0.1924	2354.471	346.405	3
3N/O	2.08(2)	3(1)	6(2)	0.0918	1123.192	165.251	3
4N/O	2.08(1)	5(1)	5(2)	0.0568	694.768	102.219	3
5N/O	2.08(1)	7(1)	5(2)	0.0616	753.883	110.916	3
6N/O	2.08(2)	9(1)	4(2)	0.0899	1100.323	161.887	3
7N/O	2.08(2)	11(2)	3(2)	0.1306	1597.774	235.075	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.19(3)	6(1)	neg13(6)	0.1533	1875.532	275.940	3
3S	2.19(2)	8(1)	neg13(4)	0.0941	1151.652	169.438	3
4S	2.19(2)	11(1)	neg13(3)	0.0800	978.594	143.977	3
5S	2.19(2)	13(1)	neg14(3)	0.0868	1061.558	156.183	3
6S	2.19(2)	15(1)	neg14(4)	0.1032	1263.109	185.837	3
7S	2.19(3)	16(2)	neg15(4)	0.1238	1515.267	222.936	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.03(2)	1(1)					
1N/O	2.16(2)	4(2)	5(2)	0.0496	607.407	126.626	5
2N/O	2.01(3)	2(3)					
2N/O	2.13(2)	1(3)	4(2)	0.0487	595.957	124.239	5
3N/O	2.04(2)	3(2)					
1N/O	2.16(3)	1(3)	4(2)	0.0450	551.188	114.906	5
4N/O	2.05(4)	8(4)					
1N/O	2.11(6)	1(4)	3(3)	0.0587	717.997	149.680	5
3N/O	2.10(3)	3(4)					
2N/O	2.00(6)	6(9)	3(2)	0.0553	676.191	140.965	5
5N/O	2.06(5)	13(4)					
1N/O	2.09(3)	1(3)	3(3)	0.0772	945.087	197.021	5
4N/O	2.08(2)	5(2)					
2N/O	1.97(0.10)	19(24)	2(3)	0.0621	759.472	158.326	5

3N/O	2.08(2)	4(2)					
3N/O	2.01(8)	17(14)	1(3)	0.0670	819.636	170.869	5
6N/O	2.09(1)	9(1)					
1N/O	2.46(3)	2(3)	5(2)	0.0349	427.547	89.130	5
5N/O	2.08(2)	7(1)					
2N/O	1.65(0.22)	65(56)	6(3)	0.0527	645.439	134.554	5
4N/O	2.10(1)	5(1)					
3N/O	2.44(6)	25(14)	8(2)	0.0462	564.970	117.779	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.15(4)	5(3)					
1S	2.27(5)	3(5)	neg13(5)	0.0870	1064.147	221.842	5
2S	2.21(0.22)	15(13)					
2S	2.18(5)	8(4)	neg13(8)	0.0793	969.955	202.206	5
3S	2.19(3)	8(3)					
1S	2.31(0.24)	17(41)	neg12(6)	0.0768	939.717	195.902	5
4S	2.19(3)	10(1)					
1S	1.45(0.32)	47(79)	neg14(5)	0.0768	939.669	195.892	5
3S	2.19(2)	8(2)					
2S	2.36(0.10)	21(22)	neg10(5)	0.0660	807.391	168.316	5
5S	2.19(2)	13(1)					
1S	3.52(0.10)	1(10)	neg14(4)	0.0721	882.476	183.969	5
4S	2.21(2)	10(1)					
2S	2.44(5)	16(9)	neg9(4)	0.0535	654.119	136.364	5
3S	2.36(8)	23(18)					
3S	2.20(2)	8(2)	neg10(5)	0.0626	765.564	159.596	5
6S	2.19(3)	14(2)					
1S	1.30(0.28)	38(54)	neg15(5)	0.0965	1180.649	246.129	5
5S	2.17(3)	11(2)					
2S	1.99(6)	19(15)	neg19(5)	0.0765	935.719	195.069	5
4S	2.21(2)	10(1)					
3S	2.44(4)	19(7)	neg8(3)	0.0444	542.861	113.170	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(3)	3(2)					5
1S	2.26(3)	3(2)	neg2(5)	0.0810	991.100	206.614	
1N/O	1.98(6)	2(4)					5
2S	2.22(3)	6(2)	neg8(6)	0.0933	1141.781	238.026	
2N/O	2.01(6)	7(5)					
2S	2.23(4)	8(3)	neg6(6)	0.0821	1004.900	209.491	5
3N/O	2.04(4)	6(2)					
1S	2.26(3)	6(4)	0(4)	0.0627	767.540	160.008	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.08(3)	7(4)					
1S	2.24(4)	10(8)	2(4)	0.0512	626.391	130.583	5
2N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.05(4)	7(5)					
2S	2.24(4)	11(6)	neg2(6)	0.0758	927.321	193.318	5
5N/O	2.10(3)	8(6)					
1S	2.20(7)	9(10)	4(3)	0.0419	513.006	106.946	5
1N/O	2.33(9)	3(7)					
5S	2.20(4)	13(3)	neg14(6)	0.0795	972.231	202.680	5
4N/O	2.08(2)	6(3)					
2S	2.23(4)	17(11)	1(4)	0.0649	794.069	165.539	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
3N/O	1.90(0.23)	27(23)					
3S	2.19(3)	8(2)	neg13(7)	0.0745	911.348	189.988	5
6N/O	2.12(3)	11(4)					
1S	2.21(4)	6(3)	5(3)	0.0423	517.399	107.862	5
1N/O	2.34(5)	1(5)					
6S	2.20(4)	15(2)	neg14(5)	0.0812	993.386	207.090	5
5N/O	2.09(2)	7(2)	2(3)	0.0542	662.956	138.206	5

2S	2.19(5)	19(13)					
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.07(2)	6(2)					
3S	2.22(5)	22(12)	neg1(5)	0.0735	899.370	187.491	5
3N/O	1.80(0.16)	32(37)					
4S	2.18(3)	10(2)	neg15(6)	0.0734	897.754	187.154	5

Table F.8. Additional Fits for Ni(II) E34C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	1(1)	7(3)	0.2401	3153.740	187.747	3
3N/O	2.08(1)	3(1)	6(2)	0.1438	1888.576	112.430	3
4N/O	2.08(1)	5(1)	5(2)	0.1101	1445.766	86.069	3
5N/O	2.08(1)	7(1)	5(1)	0.1144	1502.774	89.462	3
6N/O	2.08(1)	9(1)	4(2)	0.1413	1855.274	110.447	3
7N/O	2.08(2)	11(1)	3(2)	0.1800	2363.790	140.720	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.19(2)	6(1)	-12(4)	0.2047	2688.990	160.079	3
3S	2.19(2)	8(1)	-13(3)	0.1485	1950.628	116.124	3
4S	2.19(2)	11(1)	-13(3)	0.1351	1774.522	105.640	3
5S	2.19(2)	13(1)	-14(3)	0.1416	1859.150	110.678	3
6S	2.19(2)	15(1)	-14(3)	0.1572	2064.233	122.887	3
7S	2.19(2)	17(1)	-14(3)	0.1767	2320.925	138.168	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.03(1)	1(1)					
1N/O	2.16(1)	4(1)	5(2)	0.1028	1350.516	91.264	5
2N/O	2.01(2)	2(2)					
2N/O	2.13(2)	1(2)	4(2)	0.1026	1347.648	91.071	5
3N/O	2.04(2)	3(2)					
1N/O	2.16(2)	1(2)	4(2)	0.0984	1292.020	87.311	5

4N/O	2.05(3)	8(4)					
1N/O	2.11(5)	2(3)	3(2)	0.1127	1480.708	100.062	5
3N/O	2.11(3)	3(3)					
2N/O	2.00(4)	5(7)	3(2)	0.1094	1437.177	97.121	5
5N/O	2.06(4)	13(3)					
1N/O	2.09(3)	1(2)	3(2)	0.1313	1724.938	116.567	5
4N/O	2.08(1)	5(1)					
2N/O	1.98(9)	22(24)	2(3)	0.1159	1522.431	102.882	5
3N/O	2.08(2)	4(1)					
3N/O	2.01(7)	18(11)	2(3)	0.1210	1589.449	107.411	5
6N/O	2.09(1)	9(1)					
1N/O	2.46(2)	2(3)	5(1)	0.0898	1179.760	79.725	5
5N/O	2.08(1)	7(1)					
2N/O	1.64(0.16)	63(43)	6(3)	0.1049	1377.269	93.072	5
4N/O	2.10(1)	5(1)					
3N/O	2.44(5)	24(11)	9(1)	0.0987	1296.654	87.624	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.15(3)	5(2)					
1S	2.27(4)	3(3)	-13(4)	0.1410	1851.277	125.104	5
2S	2.21(0.16)	15(10)					
2S	2.18(4)	8(3)	-13(6)	0.1345	1767.106	119.416	5
3S	2.19(2)	8(2)					
1S	2.31(0.17)	17(31)	-12(5)	0.1319	1731.815	117.032	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.19(2)	8(2)					
2S	2.36(8)	21(16)	-10(4)	0.1212	1592.036	107.586	5
5S	2.17(2)	11(2)					
1S	1.96(6)	14(10)	-17(4)	0.1321	1735.547	117.284	5
4S	2.21(2)	10(1)					
2S	2.44(4)	16(8)	-9(3)	0.1089	1430.467	96.667	5
3S	2.36(6)	23(14)	-10(4)	0.1182	1552.429	104.909	5

3S	2.20(2)	8(1)					
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.17(2)	11(2)					
2S	1.99(5)	20(12)	-18(4)	0.1329	1745.957	117.987	5
4S	2.21(2)	10(1)					
3S	2.44(4)	19(6)	-7(3)	0.0998	1310.764	88.578	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(3)	3(2)					5
1S	2.26(2)	3(2)	-2(4)	0.1344	1764.838	119.263	
1N/O	1.98(4)	2(3)					5
2S	2.22(2)	6(2)	-8(4)	0.1463	1921.097	129.823	
2N/O	2.01(5)	6(4)					
2S	2.23(3)	8(2)	-6(4)	0.1359	1785.277	120.644	5
3N/O	2.04(3)	6(2)					
1S	2.26(3)	6(3)	-1(3)	0.1177	1545.655	104.451	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O	2.72(5)	3(5)					
4S	2.20(2)	11(1)	-12(3)	0.1139	1495.943	101.092	5
4N/O	2.08(2)	7(3)					
1S	2.24(3)	10(7)	3(3)	0.1075	1411.896	95.412	5
2N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.05(3)	7(4)					
2S	2.24(3)	11(4)	-3(4)	0.1305	1713.328	115.782	5
5N/O	2.10(3)	8(5)					
1S	2.20(7)	9(10)	5(2)	0.0986	1294.673	87.491	5
1N/O	2.33(7)	3(5)					
5S	2.20(3)	13(2)	-14(4)	0.1342	1763.096	119.145	5
4N/O	2.08(2)	6(2)					
2S	2.23(3)	17(9)	1(3)	0.1212	1592.014	107.584	5

2N/O 4S			No Fit	No Fit	No Fit	No Fit	5
3N/O 3S	1.92(0.18) 2.19(2)	28(17) 9(1)	-13(6)	0.1307	1716.566	116.001	5
6N/O 1S	2.12(2) 2.21(4)	11(4) 6(3)	5(2)	0.0991	1301.494	87.952	5
1N/O 6S	2.34(4) 2.21(3)	2(3) 15(2)	-14(4)	0.1359	1785.106	120.633	5
5N/O 2S	2.09(2) 2.19(4)	7(2) 21(12)	3(2)	0.1115	1464.311	98.954	5
2N/O 5S	1.74(7) 2.18(2)	21(16) 12(1)	-16(3)	0.1356	1781.290	120.375	5
4N/O 3S	2.07(2) 2.22(4)	6(2) 22(10)	-1(4)	0.1293	1697.950	114.743	5
3N/O 4S			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O 1Br	2.07(2) 2.43(3)	1(1) 10(3)	5(3)	0.1742	2287.285	154.569	5
1N/O 2Br	2.07(3) 2.43(5)	1(2) 14(3)	5(7)	0.3359	4411.749	298.134	5
2N/O 2Br	2.08(2) 2.44(3)	2(1) 16(4)	5(3)	0.1789	2349.362	158.764	5
3N/O 1Br	2.08(1) 2.42(3)	4(1) 12(3)	5(2)	0.1003	1317.964	89.065	5
1N/O 3Br	2.07(3) 2.44(5)	1(2) 17(4)	5(7)	0.3398	4463.321	301.619	5
1N/O 4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 1Br	2.08(1) 2.41(2)	6(1) 13(3)	5(2)	0.0734	963.944	65.141	5
2N/O 3Br	2.08(2) 2.44(4)	2(1) 20(4)	6(3)	0.1825	2397.076	161.988	5

3N/O	2.08(1)	4(1)					
2Br	2.43(3)	18(4)	5(2)	0.1032	1355.538	91.604	5
5N/O	2.08(1)	8(1)					
1Br	2.39(2)	12(3)	4(1)	0.0741	973.677	65.799	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.09(1)	6(1)					
2Br	2.41(2)	18(3)	5(1)	0.0740	971.363	65.642	5
2N/O	2.08(2)	2(1)					
4Br	2.45(4)	23(5)	6(3)	0.1856	2438.022	164.755	5
3N/O	2.09(1)	4(1)					
3Br	2.43(3)	22(4)	6(2)	0.1057	1387.998	93.797	5
6N/O	2.08(1)	10(1)					
1Br	2.38(2)	12(3)	4(2)	0.0907	1190.601	80.458	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.09(1)	8(1)					
2Br	2.40(2)	18(3)	5(1)	0.0734	963.457	65.108	5
2N/O	2.08(2)	2(1)					
5Br	2.45(4)	26(5)	6(3)	0.1885	2475.367	167.279	5
4N/O	2.09(1)	6(1)					
3Br	2.41(3)	22(4)	5(1)	0.0756	992.527	67.072	5
3N/O	2.09(1)	4(1)					
4Br	2.43(3)	25(4)	6(2)	0.1081	1419.594	95.932	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	6(1)					
1S	2.58(0.14)	26(29)					
1Br	2.42(4)	13(4)	5(2)	0.0677	889.366	69.493	7
3N/O	2.06(2)	4(1)					
2S	2.44(9)	26(12)					
1Br	2.41(3)	10(2)	3(2)	0.0758	995.183	77.762	7
2N/O	2.04(2)	3(2)					
3S	2.35(5)	19(5)	0(3)	0.0872	1145.216	89.485	7

1Br	2.37(3)	8(2)					
1N/O							
4S							
1Br			No Fit	No Fit	No Fit	No Fit	7
3N/O	2.07(2)	4(1)					
1S	2.41(0.10)	10(11)					
2Br	2.40(5)	13(4)	4(2)	0.0775	1017.649	79.517	7
2N/O	2.04(3)	1(2)					
1S	2.29(4)	2(2)					
3Br	2.30(6)	21(8)	0(3)	0.1077	1414.536	110.529	7
1N/O							
1S							
4Br			No Fit	No Fit	No Fit	No Fit	7

Ni-N(2.0) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.07(2)	11(2)					
1Imd	2.08(2)	3(3)	4(2)	0.0951	1249.398	84.431	5
4N/O	2.07(2)	8(2)					
1Imd	2.09(3)	3(4)					
1Imd	1.94(6)	9(9)	2(2)	0.0775	1017.341	79.493	7
3N/O	2.07(2)	5(2)					
1Imd	1.86(2)	0(3)					
1Imd	2.12(2)	4(2)					
1Imd	1.99(2)	5(2)	1(1)	0.0490	643.675	59.611	9
2N/O	2.08(2)	3(2)					
1Imd	2.16(2)	1(2)					
1Imd	1.86(0.13)	20(25)					
1Imd	1.52(5)	12(4)					
1Imd	2.02(2)	0(3)	6(2)	0.0415	545.129	61.962	11
1N/O	2.07(2)	2(2)					
1Imd	1.68(0.30)	20(39)					
1Imd	2.06(3)	13(4)					
1Imd	1.84(3)	6(6)					
1Imd	2.17(3)	10(3)					
1Imd	1.94(3)	12(4)	1(3)	0.0600	788.332	115.968	13
4N/O	2.08(2)	8(2)					
1Imd	2.08(3)	4(4)	5(1)	0.0787	1033.763	69.859	5
3N/O	2.08(2)	5(2)	3(2)	0.0662	868.828	67.889	7

1Imd	2.12(4)	2(3)					
1Imd	1.98(4)	5(5)					
2N/O	2.07(2)	2(2)					
1Imd	1.88(2)	0(3)					
1Imd	2.00(2)	5(2)					
1Imd	2.14(2)	5(2)	1(1)	0.0473	621.055	57.517	9
1N/O							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
3N/O	2.08(2)	5(2)					
1Imd	2.08(4)	5(5)	5(1)	0.0809	1062.519	71.802	5
2N/O	2.08(2)	3(2)					
1Imd	2.00(2)	0(2)					
1Imd	2.14(2)	0(2)	4(1)	0.0696	914.296	71.441	7
1N/O	2.06(2)	1(2)					
1Imd	2.15(2)	6(2)					
1Imd	2.02(2)	6(2)					
1Imd	1.91(3)	2(3)	2(2)	0.0720	945.131	87.530	9
0N/O							
1Imd	2.08(3)	14(4)					
1Imd	2.19(3)	10(3)					
1Imd	1.97(3)	13(4)					
1Imd	1.87(3)	7(5)	1(2)	0.1571	2063.611	191.113	9
2N/O	2.08(2)	3(2)					
1Imd	2.07(5)	4(5)	6(2)	0.1232	1617.573	109.311	5
1N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7
0N/O							
1Imd	1.93(3)	3(5)					
1Imd	2.04(3)	8(3)					
1Imd	2.15(2)	7(3)	2(2)	0.1866	2450.163	191.451	7

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(4)	0(2)					
2S	2.23(2)	7(2)					
1Imd	1.87(7)	7(6)	-9(4)	0.1097	1441.149	112.609	7
0N/O							
2S	2.22(2)	6(2)					
1Imd	1.96(4)	10(2)					
1Imd	1.83(6)	6(6)	-9(3)	0.1277	1677.09	131.045	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
2S	2.23(2)	6(2)					
1Imd	1.87(6)	6(7)					
1Imd	2.00(3)	1(2)	-7(3)	0.1118	1468.135	114.717	7

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
2S	2.22(2)	6(2)					
1Imd	1.98(4)	1(2)					
1Imd	1.83(6)	6(6)	-10(3)	0.1299	1706.296	133.327	7

Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(2)					
1S	2.46(8)	16(11)					
1Imd	1.95(7)	4(9)	-2(3)	0.0899	1181.057	109.379	9

1Imd	2.04(5)	0(4)					

Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(2)					
1S	2.45(9)	16(11)					
1Imd	1.95(6)	4(9)					
1Imd	2.04(5)	0(4)	-2(3)	0.0956	1255.607	116.283	9

Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(2)					
1S	2.46(8)	16(11)					
1Imd	1.95(6)	4(8)					
1Imd	2.04(5)	0(4)	-2(3)	0.0942	1236.606	114.523	9

Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(2)	5(3)					
1Br	2.75(4)	11(4)					
1Imd	2.08(4)	2(3)					
1Imd	1.96(3)	1(3)	-1(3)	0.1118	1467.938	135.947	9

Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.35(7)	4(8)					
1Br	2.34(7)	7(4)					
1Imd	1.97(4)	0(4)					
1Imd	2.08(3)	2(3)	0(3)	0.1120	1471.235	136.253	9

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(3)	8(5)					
1S	2.25(2)	8(5)					
1Imd	2.03(4)	5(4)	2(2)	0.0732	961.145	75.102	7

2N/O	2.05(4)	5(3)					
1S	2.26(2)	6(3)					
1Imd	2.03(4)	3(4)					
1Imd	1.89(6)	6(6)	-2(3)	0.0587	770.963	71.400	9
1N/O	2.04(3)	0(2)					
1S	2.28(3)	7(4)					
1Imd	1.97(3)	5(3)					
1Imd	1.84(4)	0(3)					
1Imd	2.10(3)	4(2)	-2(2)	0.0477	626.108	71.166	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(3)	7(4)					
1S	2.25(3)	9(5)					
1Imd	2.03(5)	5(5)	2(3)	0.0771	1012.143	79.087	7
2N/O	2.05(4)	4(3)					
1S	2.26(2)	6(3)					
1Imd	2.02(4)	3(4)					
1Imd	1.89(6)	6(6)	-2(3)	0.0617	810.726	75.082	9
1N/O	2.04(3)	0(2)					
1S	2.28(3)	7(4)					
1Imd	1.97(3)	5(2)					
1Imd	1.84(4)	1(3)					
1Imd	2.10(3)	4(2)	-2(2)	0.0505	663.478	75.414	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
1S	2.67(3)	10(4)					
1Imd	2.10(3)	4(4)	6(1)	0.0525	689.599	53.884	7
2N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.04(3)	0(2)					
1S	2.29(3)	8(4)					
1Imd	1.97(3)	5(2)					
1Imd	1.84(4)	1(3)					
1Imd	2.10(3)	5(2)	-3(2)	0.0550	721.904	82.055	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)	6(1)	0.0536	704.259	55.029	7

1S	2.67(3)	10(4)					
1Imd	2.10(3)	4(4)					
2N/O	2.07(2)	3(2)					
1S	2.66(3)	11(4)					
1Imd	2.16(2)	1(2)					
1Imd	2.01(2)	0(2)	5(1)	0.0507	666.220	61.699	9
1N/O	2.04(3)	0(2)					
1S	2.29(3)	8(5)					
1Imd	1.84(4)	1(3)					
1Imd	1.97(3)	6(2)					
1Imd	2.10(3)	5(2)	-3(2)	0.0567	745.026	84.683	11

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	6(2)					
1Br	2.41(2)	12(2)					
1Imd	2.08(3)	5(4)	5(1)	0.0453	595.193	46.507	7
2N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.07(2)	0(2)					
1Br	2.40(4)	14(5)					
1Imd	2.17(3)	3(4)					
1Imd	1.94(6)	1(9)					
1Imd	2.04(5)	3(6)	3(2)	0.0604	793.552	90.198	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	6(2)					
1Br	2.41(2)	13(2)					
1Imd	2.08(3)	5(4)	5(1)	0.0448	588.662	45.997	7
2N/O	2.08(2)	4(2)					
1Br	2.40(2)	13(3)					
1Imd	2.01(3)	1(2)					
1Imd	2.15(3)	1(3)	4(1)	0.0432	567.894	52.593	9
1N/O	2.07(2)	1(2)					
1Br	2.40(4)	14(5)					
1Imd	1.94(5)	1(9)					
1Imd	2.04(5)	3(6)					
1Imd	2.17(3)	3(4)	3(2)	0.0602	790.053	89.801	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	5(2)					
1Br	3.31(0.13)	19(18)					
1Imd	2.09(5)	5(6)	5(1)	0.0757	994.494	77.708	7
2N/O	2.07(2)	4(3)					
1Br	2.80(3)	12(4)					
1Imd	2.01(2)	1(2)					
1Imd	2.15(2)	2(2)	5(1)	0.0462	606.848	56.201	9
1N/O	2.07(3)	0(3)					
1Br	2.79(4)	12(4)					
1Imd	2.03(2)	5(3)					
1Imd	1.92(3)	0(5)					
1Imd	2.15(2)	5(2)	2(2)	0.0516	677.775	77.039	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	3(3)					
2S	2.25(3)	12(4)					
1Imd	1.97(6)	6(6)	-2(3)	0.0928	1219.001	95.250	7
1N/O	2.05(5)	2(4)					
2S	2.25(2)	9(3)					
1Imd	1.86(6)	7(8)					
1Imd	2.00(5)	3(5)	-5(3)	0.0788	1035.529	95.901	9
0N/O							
2S	2.26(2)	9(3)					
1Imd	1.95(3)	5(3)					
1Imd	2.08(3)	5(3)					
1Imd	1.83(4)	0(4)	-5(2)	0.0945	1240.673	114.900	9

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	3(3)					
2S	2.25(3)	12(4)					
1Imd	1.95(6)	6(6)	-3(4)	0.0981	1288.018	100.643	7
1N/O	2.05(5)	1(4)					
2S	2.25(2)	9(3)					
1Imd	1.99(6)	3(5)					
1Imd	1.86(6)	7(8)	-6(3)	0.0845	1110.015	102.800	9
0N/O							
2S	2.26(2)	9(3)					
1Imd	1.83(4)	0(4)					
1Imd	1.95(3)	6(3)					
1Imd	2.08(3)	5(3)	-5(3)	0.1021	1341.392	124.228	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	3(3)					
2S	2.69(0.10)	33(18)					
1Imd	2.09(5)	4(5)	6(2)	0.1116	1465.892	114.542	7
1N/O	2.07(2)	1(3)					
2S	2.56(0.19)	47(34)					
1Imd	2.14(2)	2(2)					
1Imd	2.00(2)	2(2)	4(2)	0.1009	1325.090	122.718	9

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	4(3)					
2Br	2.42(3)	18(3)					
1Imd	2.09(4)	4(5)	5(2)	0.0851	1117.774	87.341	7
1N/O							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	3(3)					
2Br	2.85(5)	18(6)					
1Imd	2.10(4)	3(4)	6(2)	0.1076	1413.393	110.440	7
1N/O	2.07(3)	1(4)					
2Br	2.82(4)	16(4)					
1Imd	2.01(2)	3(2)					
1Imd	2.15(2)	3(2)	5(2)	0.0856	1124.759	104.165	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	5(2)					
1S	2.29(3)	13(3)					
1S	2.59(3)	8(3)					
1Imd	2.03(4)	5(4)	1(2)	0.0402	528.478	48.943	9
1N/O	2.05(2)	0(2)					
1S	2.30(2)	11(3)					
1S	2.58(3)	6(2)					
1Imd	2.08(3)	2(3)					
1Imd	1.95(3)	2(3)	0(2)	0.0256	335.628	38.149	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2N/O	2.05(2)	4(3)					
1S	2.30(2)	6(2)					
1S	2.58(3)	10(4)					
1Imd	2.04(3)	5(4)	2(2)	0.0437	574.484	53.204	9
1N/O	2.03(2)	2(2)					
1S	2.30(2)	3(2)					
1S	2.55(4)	8(3)					
1Imd	1.94(3)	1(2)					
1Imd	2.08(3)	0(2)	0(2)	0.0282	370.880	42.156	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(2)	4(3)					
1S	2.29(2)	6(2)					
1S	2.58(3)	10(4)					
1Imd	2.04(3)	5(4)	2(2)	0.0429	563.826	52.216	9
1N/O	2.03(2)	2(2)					
1S	2.30(2)	3(2)					
1S	2.55(4)	8(3)					
1Imd	1.93(3)	1(2)					
1Imd	2.08(3)	0(2)	0(2)	0.0275	361.493	41.089	11

Ni-N(2.0) Ni-Br(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(2)	4(3)					
1Br	2.41(6)	10(8)					
1S	2.38(3)	8(3)					
1Imd	2.04(4)	5(4)	2(2)	0.0499	655.017	60.662	9
1N/O							
1Br							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-Br(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(2)	4(3)					
1Br	2.40(6)	10(8)					
1S	2.38(3)	8(3)					
1Imd	2.04(4)	5(4)	2(2)	0.0498	653.812	60.550	9
1N/O							
1Br							
1S			No Fit	No Fit	No Fit	No Fit	11

1Imd							
1Imd							

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(2)	2(2)					
1S	2.29(2)	3(2)					
1S	2.55(4)	9(4)					
1Imd	1.93(3)	1(2)					
1Imd	2.08(3)	1(2)	0(2)	0.0266	348.828	39.649	11

Ni-N(2.2) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	1(2)					
1S	2.29(2)	3(2)					
1S	2.56(3)	9(3)					
1Imd	1.94(3)	2(3)					
1Imd	2.08(3)	1(2)	0(2)	0.0253	284.442	32.331	11

Ni-N(2.2) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	1(2)					
1S	2.30(2)	4(2)					
1S	2.56(3)	8(3)					
1Imd	1.94(3)	1(2)					
1Imd	2.09(3)	1(2)	0(2)	0.0261	342.629	38.945	11

Ni-N(2.2) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	1(2)					
1S	2.30(2)	4(2)					
1S	2.56(3)	7(3)	0(2)	0.0269	353.496	40.180	11

1Imd	1.94(3)	1(2)					
1Imd	2.09(3)	1(2)					

Ni-N(2.2) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	1(2)					
1S	2.31(2)	4(2)					
1S	2.56(3)	7(3)					
1Imd	2.08(3)	1(2)					
1Imd	1.94(3)	1(2)	0(2)	0.0278	365.104	41.499	11

Ni-N(2.2) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	1(2)					
1S	2.30(2)	4(2)					
1S	2.56(3)	8(3)					
1Imd	2.09(3)	1(2)					
1Imd	1.94(3)	1(2)	0(2)	0.0268	351.536	39.957	11

Ni-N(2.2) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-Br(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	8(3)					
1Br	2.10(4)	1(3)					
1Br	2.31(5)	6(3)					
1Imd	2.09(2)	5(2)					
1Imd	1.94(2)	5(2)	0(2)	0.0436	572.414	65.063	11

Ni-N(2.2) Ni-Br(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	8(3)					
1Br	2.10(3)	1(3)					
1Br	2.32(4)	6(3)					
1Imd	1.94(2)	5(2)					
1Imd	2.09(2)	5(2)	0(2)	0.0432	567.433	64.497	11

Ni-N(2.2) Ni-Br(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(3)	0(3)					
1Br	2.44(6)	14(8)					
1Br	2.75(7)	13(8)					
1Imd	1.99(3)	2(2)	3(2)	0.0648	850.684	96.692	11

1Imd	2.13(3)	2(2)					

Ni-N(2.2) Ni-Br(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(3)	0(3)					
1Br	2.45(6)	14(8)					
1Br	2.75(7)	12(8)					
1Imd	2.13(3)	2(2)					
1Imd	1.99(3)	2(2)	4(2)	0.0639	839.074	95.373	11

Ni-N(2.2) Ni-Br(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(3)	0(3)					
1Br	2.45(6)	14(8)					
1Br	2.75(7)	13(8)					
1Imd	2.13(3)	2(2)					
1Imd	1.99(3)	2(2)	4(2)	0.0647	849.463	96.553	11

Ni-N(2.2) Ni-Br(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(3)	0(3)					
1Br	2.45(6)	14(8)					
1Br	2.75(7)	13(9)					
1Imd	1.99(3)	2(2)					
1Imd	2.13(3)	2(2)	4(2)	0.0645	847.507	96.331	11

Ni-N(2.2) Ni-S(2.2) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.33(7)	5(9)					
1Br	2.33(7)	8(5)					
1Imd	1.92(6)	1(10)					
1Imd	2.13(6)	3(8)					
1Imd	2.02(6)	4(7)	0(3)	0.0814	1070.188	121.642	11

Ni-N(2.2) Ni-S(2.2) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.2) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.2) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(4)	1(3)					
1S	2.28(3)	7(4)					
1Br	2.74(4)	12(4)					
1Imd	2.07(4)	1(4)					
1Imd	1.96(4)	1(4)	0(2)	0.0502	659.265	74.935	11

Ni-N(2.2) Ni-S(2.3) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.34(7)	5(9)					
1Br	2.33(7)	8(5)					
1Imd	2.13(5)	3(7)					
1Imd	1.92(6)	1(9)					
1Imd	2.02(5)	4(7)	0(2)	0.0815	1070.838	121.716	11

Ni-N(2.2) Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.33(6)	5(8)	0(2)	0.0811	1065.680	121.130	11

1Br	2.34(7)	9(5)					
1Imd	2.02(5)	4(7)					
1Imd	2.13(5)	3(7)					
1Imd	1.92(6)	1(10)					

Ni-N(2.2) Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(4)	1(3)					
1S	2.29(3)	8(5)					
1Br	2.74(4)	11(4)					
1Imd	1.96(3)	0(3)					
1Imd	2.08(4)	1(4)	0(2)	0.0531	697.688	79.302	11

Ni-N(2.2) Ni-S(2.4) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.34(6)	4(9)					
1Br	2.33(7)	7(5)					
1Imd	2.13(5)	3(7)					
1Imd	1.92(6)	1(9)					
1Imd	2.01(5)	4(7)	0(2)	0.0816	1071.521	121.794	11

Ni-N(2.2) Ni-S(2.4) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(3)	0(3)					
1S	2.29(3)	9(6)	0(2)	0.0555	729.288	82.894	11

1Br	2.74(4)	11(4)					
1Imd	2.08(4)	0(4)					
1Imd	1.96(3)	0(3)					

Ni-N(2.2) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.35(6)	4(10)					
1Br	2.33(7)	7(6)					
1Imd	2.01(5)	4(6)					
1Imd	1.91(6)	0(8)					
1Imd	2.12(5)	4(6)	0(2)	0.0821	1077.808	122.508	11

Ni-N(2.2) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	1(2)					
1S	2.38(4)	4(6)					
1Br	2.37(4)	6(3)					
1Imd	2.09(3)	0(2)					
1Imd	1.95(3)	1(2)	0(2)	0.0301	395.077	44.906	11

Ni-N(2.2) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	11

1Imd							
1Imd							
0N/O							
1S	2.35(6)	4(10)					
1Br	2.33(7)	6(6)					
1Imd	2.01(5)	4(6)					
1Imd	1.91(6)	0(8)					
1Imd	2.12(4)	4(6)	-1(2)	0.0825	1084.073	123.220	11

Ni-N(2.2) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.2) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	1(2)					
1S	2.40(5)	4(6)					
1Br	2.37(4)	6(3)					
1Imd	1.95(3)	1(2)					
1Imd	2.09(3)	0(2)	0(2)	0.0307	403.532	45.867	11

Ni-N(2.2) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	5(2)					
1S	2.29(2)	7(3)					
1S	2.58(3)	10(4)					
1Imd	1.96(7)	7(7)					
1Imd	2.08(4)	3(5)	1(2)	0.0270	354.851	40.334	11

Ni-N(2.2) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	5(2)					
1S	2.29(3)	8(4)					
1S	2.59(3)	10(3)					
1Imd	1.98(9)	9(12)	1(2)	0.0246	322.621	36.670	11

1Imd	2.07(6)	4(6)					
3N/O	2.09(3)	9(4)					
1S	2.27(3)	9(5)					
1S	2.61(3)	10(4)					
1Imd	2.05(2)	4(2)	2(1)	0.0308	405.004	37.508	9

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(3)	9(7)					
1S	2.21(6)	9(9)					
1Imd	2.06(4)	5(4)	4(2)	0.0664	871.799	68.121	7
3N/O	2.08(4)	8(5)					
1S	2.24(2)	7(4)					
1Imd	1.90(7)	8(8)					
1Imd	2.04(4)	3(4)	-1(3)	0.0560	735.345	68.101	9
2N/O	2.07(3)	4(3)					
1S	2.26(4)	11(8)					
1Imd	1.84(4)	0(3)					
1Imd	1.97(3)	4(3)					
1Imd	2.10(3)	3(3)	-1(2)	0.0420	550.992	62.628	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(4)	8(5)					
1S	2.21(6)	11(10)					
1Imd	2.06(4)	5(4)	4(2)	0.0683	897.509	70.130	7
3N/O	2.08(4)	8(4)					
1S	2.25(2)	7(4)					
1Imd	2.03(4)	3(4)					
1Imd	1.90(7)	7(7)	-1(3)	0.0583	765.083	70.855	9
2N/O	2.07(3)	4(3)					
1S	2.26(4)	12(8)					
1Imd	1.97(3)	4(2)					
1Imd	1.84(4)	0(3)					
1Imd	2.10(3)	4(3)	-2(2)	0.0433	569.050	64.681	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	8(2)					
1S	2.01(0.18)	41(44)					
1Imd	2.09(4)	4(4)	6(2)	0.0730	959.082	74.941	7
3N/O	2.09(3)	5(3)					
1S	2.19(7)	16(15)	3(2)	0.0630	827.677	76.652	9

1Imd	1.99(4)	2(4)					
1Imd	2.13(5)	2(5)					
2N/O	2.07(2)	3(3)					
1S	2.27(4)	13(9)					
1Imd	2.10(3)	4(2)					
1Imd	1.97(3)	5(2)					
1Imd	1.84(4)	0(3)	-2(2)	0.0445	584.296	66.413	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	8(2)					
1S	2.66(2)	10(3)					
1Imd	2.10(2)	4(3)	5(1)	0.0447	587.730	45.924	7
3N/O	2.07(1)	6(2)					
1S	2.65(3)	10(4)					
1Imd	2.01(4)	4(4)					
1Imd	2.15(3)	2(3)	5(1)	0.0443	581.344	53.839	9
2N/O	2.07(2)	3(2)					
1S	2.64(5)	15(8)					
1Imd	2.02(2)	4(3)					
1Imd	2.15(2)	4(2)					
1Imd	1.91(4)	2(5)	3(1)	0.0450	590.483	67.117	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	8(2)					
1S	2.67(2)	10(3)					
1Imd	2.10(2)	4(3)	5(1)	0.0461	605.016	47.275	7
3N/O	2.07(1)	6(2)					
1S	2.66(3)	10(4)					
1Imd	2.01(4)	4(4)					
1Imd	2.14(3)	2(3)	5(1)	0.0457	599.699	55.539	9
2N/O	2.07(2)	3(2)					
1S	2.64(5)	16(8)					
1Imd	2.02(2)	4(3)					
1Imd	1.90(3)	2(5)					
1Imd	2.15(2)	4(2)	2(1)	0.0451	592.877	67.389	11

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	10(2)					
1Br	2.39(2)	12(2)					
1Imd	2.07(2)	4(3)	4(1)	0.0391	513.233	40.103	7

3N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O	2.07(2)	3(2)					
1Br	2.39(4)	15(5)					
1Imd	2.02(3)	2(4)					
1Imd	2.15(3)	2(3)					
1Imd	1.90(5)	3(6)	2(2)	0.0385	505.088	57.410	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.08(2)	10(2)					
1Br	2.40(2)	12(2)					
1Imd	2.07(2)	4(3)	4(1)	0.0389	511.468	39.965	7
3N/O	2.08(2)	7(2)					
1Br	2.39(2)	13(3)					
1Imd	2.10(0.89)	8(24)					
1Imd	2.05(0.91)	9(67)	4(2)	0.0368	483.538	44.781	9
2N/O	2.07(2)	3(2)					
1Br	2.39(3)	15(5)					
1Imd	2.15(3)	2(3)					
1Imd	1.90(5)	3(6)					
1Imd	2.02(3)	2(4)	2(2)	0.0383	502.517	57.118	11

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.08(2)	10(2)					
1Br	2.40(2)	12(2)					
1Imd	2.08(2)	4(3)	4(1)	0.0390	511.876	39.997	7
3N/O	2.08(2)	7(2)					
1Br	2.40(2)	13(3)					
1Imd	2.05(0.63)	9(5)					
1Imd	2.10(0.60)	8(17)	4(2)	0.0368	483.594	44.786	9
2N/O	2.07(2)	3(2)					
1Br	2.40(3)	15(5)					
1Imd	1.90(5)	3(6)					
1Imd	2.02(3)	2(4)					
1Imd	2.15(3)	2(3)	2(2)	0.0381	500.793	56.922	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.07(2)	9(2)					
1Br	2.82(3)	13(4)	4(1)	0.0536	703.331	54.957	7

1Imd	2.09(2)	2(2)					
3N/O	2.06(2)	10(3)					
1Br	2.81(2)	10(3)					
1Imd	2.02(2)	2(2)					
1Imd	2.15(2)	3(2)	4(1)	0.0417	548.168	50.766	9
2N/O	2.07(2)	4(2)					
1Br	2.80(3)	12(4)					
1Imd	1.89(3)	2(3)					
1Imd	2.01(2)	5(2)					
1Imd	2.15(3)	2(3)	2(1)	0.2920	383.065	43.541	11

Table F.9. Additional Fits for Co(II) E34C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(3)	2(2)	5(6)	0.2810	1191.058	175.236	3
3N/O	2.14(2)	4(2)	3(4)	0.1814	769.059	113.149	3
4N/O	2.13(2)	6(2)	2(3)	0.1314	557.117	81.967	3
5N/O	2.13(2)	8(2)	1(3)	0.1115	472.630	69.536	3
6N/O	2.12(2)	9(2)	1(3)	0.1101	466.494	68.634	3
7N/O	2.12(2)	11(2)	neg1(3)	0.1199	507.986	74.738	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.24(3)	6(2)	neg15(7)	0.2178	923.289	135.840	3
3S	2.24(3)	9(2)	neg16(5)	0.1542	653.575	96.158	3
4S	2.23(3)	11(1)	neg17(5)	0.1265	536.214	78.891	3
5S	2.23(3)	13(2)	neg18(4)	0.1168	495.213	72.859	3
6S	2.23(3)	15(2)	neg19(4)	0.1168	495.171	72.853	3
7S	2.23(3)	16(2)	neg19(4)	0.1222	517.823	76.185	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.05(2)	1(1)					
1N/O	2.18(1)	5(1)	neg1(3)	0.0539	228.386	47.611	5
2N/O	2.02(1)	1(1)					
2N/O	2.16(1)	2(1)	neg2(1)	0.0226	95.592	19.928	5
3N/O	2.05(1)	2(1)					
1N/O	2.18(1)	4(1)	neg2(2)	0.0241	102.189	21.303	5
4N/O	2.06(1)	5(1)	neg3(1)	0.0201	85.022	17.724	5

1N/O	2.18(1)	3(1)					
3N/O	2.03(1)	3(1)					
2N/O	2.17(1)	1(1)	neg3(1)	0.0227	96.298	20.075	5
5N/O	2.06(1)	8(1)					
1N/O	2.17(1)	3(1)	neg4(2)	0.0296	125.649	26.194	5
4N/O	2.03(2)	6(2)					
2N/O	2.16(1)	1(1)	neg4(2)	0.0364	154.440	32.196	5
3N/O	2.00(2)	4(2)					
3N/O	2.15(1)	1(1)	neg4(2)	0.0428	181.289	37.793	5
6N/O	2.06(2)	10(2)					
1N/O	2.17(1)	2(1)	neg4(2)	0.0459	194.591	40.566	5
5N/O	2.03(2)	8(2)					
2N/O	2.16(2)	1(1)	neg5(2)	0.0559	237.118	49.432	5
4N/O	2.01(2)	7(3)					
3N/O	2.15(2)	2(2)	neg5(2)	0.0645	273.299	56.974	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.23(3)	2(1)					
1S	2.09(3)	1(2)	neg23(5)	0.0960	406.922	84.831	5
2S	2.10(3)	5(2)					
2S	2.25(2)	3(2)	neg24(5)	0.0762	322.869	67.308	5
3S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.26(3)	10(2)					
1S	2.51(6)	8(7)	neg12(5)	0.1074	455.330	94.922	5
3S	2.23(2)	5(2)					
2S	2.09(3)	6(3)	neg25(5)	0.0770	326.431	68.051	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.26(3)	9(2)					
2S	2.49(6)	14(9)	neg11(5)	0.0961	407.473	84.946	5
3S	2.09(4)	10(3)					
3S	2.24(3)	6(2)	neg26(5)	0.0820	347.763	72.498	5

6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.27(3)	11(1)					
2S	2.52(4)	11(5)	neg11(4)	0.0758	321.488	67.020	5
4S	2.26(3)	9(2)					
3S	2.49(6)	17(8)	neg11(4)	0.0856	363.024	75.679	5

Co-N(2.0) Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	3(2)					5
1S	2.27(2)	1(1)	neg12(5)	0.0814	344.828	71.886	
1N/O	2.70(0.13)	5(16)					5
2S	2.25(3)	6(2)	neg13(7)	0.1942	823.143	171.600	
2N/O	1.96(4)	5(3)					
2S	2.25(2)	5(1)	neg16(4)	0.0722	306.223	63.838	5
3N/O	2.01(3)	6(2)					
1S	2.27(2)	2(1)	neg11(4)	0.0637	269.800	56.245	5
1N/O	1.93(3)	2(3)					
3S	2.24(2)	7(1)	neg18(4)	0.0762	323.156	67.368	5
1N/O	1.91(4)	3(4)					
4S	2.23(3)	10(1)	neg19(4)	0.0869	368.234	76.765	5
4N/O	2.02(4)	9(3)					
1S	2.28(2)	2(1)	neg11(4)	0.0574	243.418	50.745	5
2N/O	1.94(5)	7(4)					
3S	2.24(3)	8(2)	neg17(5)	0.0838	355.240	74.056	5
3N/O	1.97(5)	9(4)					
2S	2.26(3)	6(2)	neg15(5)	0.0742	314.397	65.542	5
5N/O	2.04(5)	12(3)					
1S	2.28(2)	3(2)	neg10(5)	0.0558	236.579	49.319	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.99(7)	13(5)					
2S	2.26(3)	6(2)	neg14(6)	0.0774	328.217	68.423	5
2N/O	1.92(9)	11(8)					
4S	2.24(3)	11(2)	neg18(6)	0.0984	417.147	86.962	5

3N/O	1.95(8)	13(7)					
3S	2.25(3)	9(2)	neg17(6)	0.0901	381.984	79.632	5
6N/O	2.06(6)	15(3)					
1S	2.28(2)	3(2)	neg8(5)	0.0552	234.080	48.798	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.01(9)	17(5)					
2S	2.26(3)	7(2)	neg13(7)	0.1154	488.918	101.924	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.98(0.13)	18(9)					
3S	2.25(4)	9(3)	neg16(8)	0.0929	393.740	82.083	5
3N/O	1.94(0.17)	19(15)					
4S	2.24(4)	11(3)	neg18(8)	0.1017	431.113	89.874	5

Table F.10. Additional Fits for Co(II) E34C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	2(1)	5(4)	0.3231	1464.535	87.186	3
3N/O	2.14(2)	4(1)	4(3)	0.2291	1038.399	61.817	3
4N/O	2.13(2)	6(1)	2(2)	0.1818	824.120	49.061	3
5N/O	2.13(2)	8(1)	1(2)	0.1631	739.243	44.008	3
6N/O	2.12(2)	10(1)	1(2)	0.1620	734.166	43.706	3
7N/O	2.12(2)	11(1)	-1(2)	0.1716	777.705	46.298	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.24(2)	6(1)	-14(5)	0.2609	1182.813	70.415	3
3S	2.24(2)	9(1)	-16(4)	0.2020	915.943	54.527	3
4S	2.23(2)	11(1)	-17(4)	0.1766	800.411	47.650	3
5S	2.23(2)	13(1)	-18(3)	0.1678	760.748	45.288	3
6S	2.23(2)	15(1)	-19(3)	0.1681	761.837	45.353	3
7S	2.23(2)	16(1)	-19(3)	0.1733	785.503	46.762	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar

2N/O	2.05(1)	1(1)					
1N/O	2.18(1)	5(1)	-1(2)	0.0922	417.814	28.235	5
2N/O	2.02(1)	1(1)					
2N/O	2.16(1)	2(1)	-2(1)	0.0654	296.676	20.049	5
3N/O	2.05(1)	2(1)					
1N/O	2.18(1)	4(1)	-2(2)	0.0650	294.565	19.906	5
4N/O	2.06(1)	5(1)					
1N/O	2.18(1)	3(1)	-3(1)	0.0631	286.017	19.328	5
3N/O	2.03(1)	3(1)					
2N/O	2.17(1)	1(1)	-3(1)	0.0746	338.071	22.846	5
5N/O	2.06(1)	7(1)					
1N/O	2.18(1)	3(1)	-4(2)	0.0674	305.582	20.650	5
4N/O	2.03(1)	5(1)					
2N/O	2.17(1)	1(1)	-4(2)	0.0830	376.117	25.417	5
3N/O	2.00(1)	3(1)					
3N/O	2.15(1)	1(1)	-4(2)	0.0910	412.719	27.890	5
6N/O	2.06(2)	10(1)					
1N/O	2.17(1)	2(1)	-4(2)	0.0926	419.651	28.359	5
5N/O	2.03(2)	8(2)					
2N/O	2.16(1)	1(1)	-5(2)	0.1043	472.933	31.960	5
4N/O	2.01(2)	6(2)					
3N/O	2.15(1)	2(1)	-5(2)	0.1144	418.448	35.035	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.23(2)	2(1)					
1S	2.09(2)	1(1)	-23(4)	0.1365	618.688	41.809	5
2S	2.25(2)	2(1)					
2S	2.10(2)	5(2)	-24(3)	0.1234	559.363	37.800	5
3S	2.22(2)	4(1)					
1S	2.07(2)	2(1)	-23(3)	0.1220	552.946	37.367	5
4S	2.27(2)	10(1)					
1S	2.52(3)	7(4)	-12(4)	0.1546	700.966	47.369	5
3S	2.24(2)	5(1)					
2S	2.08(2)	6(2)	-25(3)	0.1668	755.949	51.085	5

5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.26(2)	9(1)					
2S	2.50(4)	13(6)	-11(3)	0.1455	659.804	44.588	5
3S	2.24(2)	5(1)					
3S	2.09(3)	9(2)	-26(4)	0.1304	591.121	39.946	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.26(2)	9(1)					
3S	2.49(4)	17(6)	-10(3)	0.1358	615.728	41.609	5

Co-N(2.0) Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	3(2)					5
1S	2.27(2)	1(1)	-12(3)	0.1207	547.329	36.987	
1N/O	2.69(6)	3(6)					5
2S	2.25(2)	6(1)	-13(4)	0.2355	1067.393	72.130	
2N/O	1.96(2)	5(2)					
2S	2.25(2)	5(1)	-15(3)	0.1178	534.216	36.101	5
3N/O	2.01(2)	6(2)					
1S	2.27(1)	1(1)	-12(3)	0.1062	481.419	32.533	5
1N/O	1.93(2)	1(2)					
3S	2.24(2)	7(1)	-17(3)	0.1236	560.216	37.858	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.02(3)	9(2)					
1S	2.28(1)	2(1)	-11(3)	0.1024	464.391	31.382	5
2N/O	1.94(3)	7(3)					
3S	2.25(2)	8(1)	-17(3)	0.1219	552.472	37.335	5
3N/O	1.97(3)	8(3)					
2S	2.26(2)	5(1)	-15(3)	0.1331	603.321	40.771	5
5N/O	2.03(3)	12(2)	-10(3)	0.1028	466.071	31.496	5

1S	2.28(2)	3(1)					
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.99(5)	12(3)					
2S	2.26(2)	6(1)	-14(4)	0.1495	677.643	45.793	5
2N/O	1.92(6)	10(5)					
4S	2.24(2)	11(2)	-18(4)	0.1266	573.801	38.776	5
3N/O	1.95(6)	12(5)					
3S	2.25(2)	9(2)	-17(4)	0.1406	637.176	43.059	5
6N/O	2.05(4)	15(2)					
1S	2.28(2)	3(1)	-9(4)	0.1039	471.104	31.836	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.01(7)	16(4)					
2S	2.26(2)	7(2)	-13(5)	0.1656	750.744	50.733	5
2N/O	1.31(0.34)	40(55)					
5S	2.23(3)	13(1)	-18(4)	0.1295	586.953	39.665	5
4N/O	1.98(9)	18(6)					
3S	2.25(3)	9(2)	-16(5)	0.1439	652.228	44.076	5
3N/O	1.94(0.12)	19(11)					
4S	2.24(3)	11(2)	-18(6)	0.1532	694.380	46.924	5

Co-N(2.0) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.13(1)	5(1)					
1Imd	1.97(2)	1(2)	-2(2)	0.1265	573.277	38.741	5
4N/O	2.12(2)	7(2)					
1Imd	2.16(2)	1(2)					
1Imd	1.99(2)	0(1)	-2(1)	0.0647	293.405	22.926	7
3N/O	2.12(2)	4(2)					
1Imd	2.01(5)	2(4)					
1Imd	2.16(2)	2(3)					
1Imd	1.94(7)	5(13)	-3(2)	0.0556	252.224	23.359	9
2N/O	2.13(2)	2(2)					
1Imd	2.35(8)	2(11)					
1Imd	2.08(4)	8(5)	-1(2)	0.0585	265.165	30.140	11

1Imd	2.21(4)	7(5)					
1Imd	1.96(3)	5(4)					
1N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13
4N/O	2.13(1)	3(1)					
1Imd	1.98(2)	0(1)	-1(2)	0.1208	547.640	37.008	5
3N/O	2.12(2)	4(2)					
1Imd	2.15(2)	1(2)					
1Imd	1.99(2)	1(1)	-1(1)	0.0610	276.622	21.615	7
2N/O	2.13(2)	2(2)					
1Imd	2.05(6)	2(12)					
1Imd	1.96(8)	0(10)					
1Imd	2.18(3)	2(5)	-2(2)	0.0640	289.970	26.854	9
1N/O	2.13(2)	2(2)					
1Imd	2.19(0.71)	6(120)					
1Imd	2.04(0.23)	4(26)					
1Imd	2.17(0.38)	3(19)					
1Imd	1.95(0.16)	2(21)	-2(3)	0.0841	381.098	43.317	11
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
3N/O	2.14(1)	1(1)					
1Imd	2.00(2)	0(1)	-1(2)	0.1369	620.466	41.929	5
2N/O	2.13(2)	2(2)					
1Imd	2.15(2)	2(2)					
1Imd	2.00(1)	2(1)	-1(2)	0.0794	359.777	28.112	7
1N/O	2.13(2)	2(2)					
1Imd	2.20(3)	5(3)					
1Imd	2.07(3)	6(4)					
1Imd	1.96(3)	4(3)	-2(2)	0.0944	428.079	39.645	9
0N/O							
1Imd	2.23(9)	6(19)					
1Imd	2.03(8)	9(15)	-3(3)	0.1972	893.819	82.777	9

1Imd	2.14(8)	10(18)					
1Imd	1.94(7)	5(11)					
2N/O	2.15(2)	1(1)					
1Imd	2.02(2)	1(2)	-1(3)	0.1863	844.591	57.075	5
1N/O	2.14(2)	2(2)					
1Imd	2.16(2)	2(2)					
1Imd	2.01(2)	3(1)	-1(2)	0.1366	619.347	48.395	7
0N/O							
1Imd	1.97(3)	6(4)					
1Imd	2.19(2)	8(3)					
1Imd	2.08(3)	9(4)	-2(3)	0.2238	1014.691	79.286	7

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(5)	6(5)					
1S	2.28(1)	2(1)					
1Imd	1.97(4)	4(4)	-10(3)	0.0886	401.729	31.390	7
1N/O	2.10(5)	1(4)					
1S	2.30(3)	5(3)					
1Imd	1.97(2)	1(2)					
1Imd	2.12(4)	0(3)	-6(3)	0.0850	385.211	35.675	9
0N/O							
1S	2.29(2)	3(2)					
1Imd	2.12(9)	0(7)					
1Imd	2.05(0.46)	12(40)					
1Imd	1.98(6)	0(5)	-7(5)	0.1175	532.457	49.311	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(5)	5(5)					
1S	2.28(1)	2(1)					
1Imd	1.97(5)	4(4)	neg10(3)	0.0926	419.676	32.793	7
1N/O	2.10(4)	1(4)					
1S	2.31(3)	5(3)					
1Imd	2.12(4)	0(3)					
1Imd	1.97(2)	1(2)	neg6(3)	0.0899	407.564	37.745	9
0N/O							
1S	2.29(2)	3(2)					
1Imd	2.13(6)	3(6)					
1Imd	2.00(7)	2(6)					
1Imd	1.94(0.15)	6(24)	neg8(4)	0.1235	559.658	51.830	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(5)	5(5)					
1S	2.28(1)	2(1)					
1Imd	1.96(5)	4(4)	neg11(3)	0.0954	432.487	33.794	7
1N/O	2.10(4)	1(4)					
1S	2.31(3)	6(3)					
1Imd	2.12(4)	0(3)					
1Imd	1.97(2)	2(2)	neg6(3)	0.0939	425.534	39.409	9
0N/O							
1S	2.29(2)	3(3)					
1Imd	1.99(6)	3(6)					
1Imd	2.12(5)	3(5)					
1Imd	1.93(0.12)	5(19)	neg9(4)	0.1280	580.122	53.726	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(5)	5(5)					
1S	2.28(2)	2(1)					
1Imd	1.96(5)	4(4)	neg11(4)	0.0978	443.566	34.659	7
1N/O	2.11(4)	1(3)					
1S	2.31(3)	6(4)					
1Imd	2.12(4)	0(3)					
1Imd	1.97(2)	2(2)	neg6(3)	0.0975	442.046	40.938	9
0N/O							
1S	2.29(2)	3(3)					
1Imd	1.92(0.11)	5(17)					
1Imd	1.99(5)	3(6)					
1Imd	2.12(5)	3(5)	neg9(4)	0.1318	597.336	55.320	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(5)	5(5)					
1S	2.28(2)	2(1)					
1Imd	1.96(5)	4(5)	neg12(4)	0.0997	452.152	35.330	7
1N/O	2.11(4)	1(3)					
1S	2.31(3)	7(4)					
1Imd	2.12(4)	0(3)					
1Imd	1.97(2)	2(2)	neg6(3)	0.1005	455.664	42.199	9
0N/O							
1S	2.29(2)	3(3)					
1Imd	1.99(5)	3(5)					
1Imd	2.12(5)	3(5)					
1Imd	1.91(0.11)	5(16)	neg9(4)	0.1346	610.152	56.507	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	1(1)					
1Br	2.44(6)	15(7)					
1Imd	2.01(3)	0(2)	neg1(3)	0.1729	783.609	61.230	7
1N/O	2.13(3)	1(3)					
1Br	2.44(5)	15(7)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(3)	2(2)	neg1(3)	0.1269	575.111	53.262	9
0N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	1(1)					
1Br	2.44(6)	15(7)					
1Imd	2.01(3)	0(2)	neg1(3)	0.1731	784.686	61.314	7
1N/O	2.13(3)	1(3)					
1Br	2.44(5)	15(7)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(3)	2(2)	neg1(3)	0.1267	574.271	53.184	9
0N/O							
1Br	2.42(4)	11(5)					
1Imd	2.12(5)	7(6)					
1Imd	1.99(3)	5(4)					
1Imd	2.22(6)	4(9)	neg1(3)	0.2004	908.316	84.120	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	1(1)					
1Br	2.44(6)	16(7)					
1Imd	2.01(3)	0(2)	neg1(3)	0.1730	784.404	61.292	7
1N/O	2.13(3)	1(3)					
1Br	2.44(5)	16(7)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(3)	2(2)	neg1(3)	0.1262	572.068	52.980	9
0N/O							
1Br	2.42(4)	11(5)					
1Imd	2.22(4)	4(9)	neg1(3)	0.2001	907.109	84.008	11

1Imd	1.99(3)	5(4)					
1Imd	2.11(5)	7(6)					

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	1(1)					
1Br	2.44(6)	16(7)					
1Imd	2.01(3)	0(2)	neg1(3)	0.1728	783.492	61.221	7
1N/O	2.13(3)	1(3)					
1Br	2.45(5)	16(7)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(3)	2(2)	neg1(3)	0.1257	569.733	52.764	9
0N/O							
1Br	2.43(4)	11(5)					
1Imd	1.99(3)	5(4)					
1Imd	2.22(5)	4(9)					
1Imd	2.11(5)	7(6)	neg1(3)	0.1998	905.719	83.880	11

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(9)	6(10)					
2S	2.26(2)	5(1)					
1Imd	1.95(4)	3(4)	neg14(3)	0.1085	491.741	38.424	7
0N/O							
2S	2.25(2)	5(1)					
1Imd	1.96(2)	1(2)					
1Imd	1.87(0.14)	18(29)	neg15(4)	0.1203	545.29	42.608	9

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(9)	6(9)					
2S	2.26(2)	5(1)					
1Imd	1.95(4)	4(4)	neg14(3)	0.1126	510.573	39.895	7
0N/O							
2S	2.25(2)	5(1)					
1Imd	1.96(2)	1(2)					
1Imd	1.85(0.12)	17(24)	neg16(4)	0.1229	557.115	43.532	9

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	1(2)					
2S	2.24(2)	4(1)					
1Imd	1.87(9)	12(13)	neg18(3)	0.1097	497.378	38.864	7
0N/O			neg17(4)	0.1237	560.926	43.830	9

2S	2.25(2)	5(1)					
1Imd	1.83(0.10)	15(20)					
1Imd	1.95(2)	1(2)					

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	1(2)					
2S	2.24(2)	4(1)					
1Imd	1.86(8)	12(13)	neg19(3)	0.1094	495.937	38.752	7
0N/O							
2S	2.24(2)	5(1)					
1Imd	1.82(9)	14(17)					
1Imd	1.95(2)	1(2)	neg18(4)	0.1234	559.274	43.701	9

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	0(2)					
2S	2.24(2)	5(1)					
1Imd	1.86(8)	12(13)	neg19(3)	0.1092	495.139	38.689	7
0N/O							
2S	2.24(2)	5(1)					
1Imd	1.95(2)	1(2)					
1Imd	1.81(8)	13(15)	neg18(4)	0.1228	556.754	43.504	9

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.15(2)	4(2)					
2Br	2.46(6)	19(7)					
1Imd	2.03(3)	1(2)	neg2(5)	0.2620	1187.943	92.824	7
0N/O							
2Br	2.45(5)	17(6)					
1Imd	2.16(2)	4(2)					
1Imd	2.02(3)	3(2)	neg2(4)	0.2755	1249.057	97.599	9

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(2)	4(2)					
2Br	2.47(7)	19(8)					
1Imd	2.03(3)	1(2)	neg1(5)	0.2630	1192.165	93.153	7
0N/O							
2Br	2.46(5)	17(6)					
1Imd	2.02(3)	3(2)					
1Imd	2.16(2)	4(2)	neg2(4)	0.2763	1252.746	97.887	9

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.17(3)	2(2)					
2Br	2.55(0.10)	23(13)					
1Imd	1.62(7)	12(8)	9(6)	0.3196	1448.762	113.204	7
0N/O							
2Br	2.46(5)	18(6)					
1Imd	2.02(3)	3(2)					
1Imd	2.16(2)	4(2)	neg2(3)	0.2761	1251.711	97.806	9

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(2)	4(2)					
2Br	2.47(7)	20(8)					
1Imd	2.03(3)	1(2)	neg1(4)	0.2628	1191.414	93.095	7
0N/O							
2Br	2.46(5)	18(6)					
1Imd	2.16(2)	5(2)					
1Imd	2.02(3)	3(2)	neg2(3)	0.2757	1249.83	97.659	9

Co-N(2.0) Co-S(2.2) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(5)	3(4)					
1S	2.27(3)	3(3)					
1Br	2.19(6)	5(7)					
1Imd	1.99(5)	4(5)	neg9(4)	0.0878	398.169	36.875	9
0N/O							
1S	2.36(6)	1(5)					
1Br	2.34(7)	6(5)					
1Imd	2.12(2)	3(2)					
1Imd	1.99(2)	3(2)	neg5(3)	0.1163	527.165	48.821	11

Co-N(2.0) Co-S(2.3) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(5)	3(4)					
1S	2.27(3)	2(3)					
1Br	2.20(6)	6(7)					
1Imd	1.99(5)	4(5)	neg9(4)	0.0844	382.661	35.439	9
0N/O							
1S	2.34(6)	2(4)					
1Br	2.34(7)	7(5)					
1Imd	1.99(2)	3(2)					
1Imd	2.12(3)	3(2)	neg5(3)	0.1149	520.75	48.227	11

Co-N(2.0) Co-S(2.4) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	2.04(5)	3(4)					
1S	2.27(4)	3(4)					
1Br	2.20(6)	4(7)					
1Imd	1.98(5)	3(5)	neg10(4)	0.0935	423.764	39.245	9
0N/O							
1S	2.38(6)	1(6)					
1Br	2.35(6)	3(5)					
1Imd	1.98(2)	3(2)					
1Imd	2.12(2)	3(2)	neg5(3)	0.1127	510.705	47.297	11

Co-N(2.0) Co-S(2.4) Co-Br(2.5) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O	2.04(5)	3(4)					
1S	2.27(3)	2(3)					
1Br	2.20(6)	6(7)					
1Imd	1.98(5)	4(5)	neg10(4)	0.0893	404.64	37.474	9
0N/O							
1S	2.37(6)	1(5)					
1Br	2.35(6)	5(4)					
1Imd	2.12(2)	3(2)					
1Imd	1.98(2)	3(2)	neg5(3)	0.1138	515.904	47.778	11

Co-N(2.0) Co-S(2.6) Co-Br(2.3) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O	2.04(6)	3(4)					
1S	2.27(4)	3(4)					
1Br	2.19(7)	4(8)					
1Imd	2.04(5)	4(5)	neg11(5)	0.0972	440.827	40.825	9
0N/O							
1S	2.41(3)	9(3)					
1Br	2.36(3)	5(3)					
1Imd	2.14(2)	5(2)					
1Imd	1.98(2)	5(2)	neg4(2)	0.1005	455.431	42.178	11

Co-N(2.0) Co-S(2.6) Co-Br(2.5) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O	2.03(5)	3(4)					
1S	2.27(4)	2(3)					
1Br	2.20(6)	6(7)					
1Imd	1.97(5)	4(5)	neg11(4)	0.0925	419.444	38.845	9
0N/O							
1S	2.38(6)	1(6)					
1Br	2.35(6)	4(4)					
1Imd	2.12(2)	3(2)					
1Imd	1.98(2)	3(2)	neg5(3)	0.1124	509.461	47.182	11

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(5)	10(5)					
1S	2.28(1)	2(1)					
1Imd	1.98(3)	4(3)	neg8(3)	0.0785	355.783	27.800	7
2N/O	2.13(2)	3(3)					
1S	2.29(4)	11(7)					
1Imd	2.14(3)	1(3)					
1Imd	1.98(2)	1(1)	neg4(2)	0.0667	302.523	28.017	9
1N/O	2.10(6)	1(4)					
1S	2.31(3)	6(5)					
1Imd	1.91(0.11)	5(13)					
1Imd	2.13(5)	3(4)					
1Imd	1.99(5)	3(4)	neg7(4)	0.0715	323.984	36.825	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(5)	10(5)					
1S	2.28(1)	2(1)					
1Imd	1.98(4)	4(3)	neg9(3)	0.0826	374.446	29.259	7
2N/O	2.13(2)	2(2)					
1S	2.30(5)	13(8)					
1Imd	1.98(2)	2(1)					
1Imd	2.14(3)	1(2)	neg3(2)	0.0698	316.197	29.283	9
1N/O	2.11(5)	1(3)					
1S	2.31(4)	7(6)					
1Imd	2.14(5)	3(4)					
1Imd	2.00(6)	3(5)					
1Imd	1.93(0.11)	4(14)	neg6(4)	0.0748	338.894	38.520	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(5)	10(5)					
1S	2.28(1)	2(1)					
1Imd	1.97(4)	4(3)	neg9(3)	0.0858	388.812	30.381	7
2N/O	2.03(5)	5(5)					
1S	2.28(2)	1(1)					
1Imd	1.86(0.13)	16(25)					
1Imd	1.97(5)	4(4)	neg12(4)	0.0860	389.732	36.093	9
1N/O	2.12(4)	1(3)					
1S	2.32(4)	9(8)					
1Imd	2.01(7)	3(5)	neg6(4)	0.0772	350.184	39.803	11

1Imd	2.15(6)	3(4)					
1Imd	1.94(0.11)	3(15)					

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(5)	10(5)					
1S	2.28(1)	3(1)					
1Imd	1.97(4)	4(3)	neg10(3)	0.0886	401.430	31.367	7
2N/O	2.13(2)	2(2)					
1S	2.47(0.18)	34(30)					
1Imd	2.15(2)	2(2)					
1Imd	1.99(2)	2(1)	neg2(2)	0.0704	318.969	29.540	9
1N/O	2.13(2)	2(2)					
1S	2.42(0.12)	25(24)					
1Imd	1.95(4)	3(5)					
1Imd	2.06(4)	6(5)					
1Imd	2.18(4)	5(4)	neg3(2)	0.0779	353.311	40.159	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(5)	9(5)					
1S	2.28(2)	3(1)					
1Imd	1.97(4)	4(3)	neg10(3)	0.0908	411.420	32.148	7
2N/O	2.13(2)	2(2)					
1S	2.49(0.19)	35(31)					
1Imd	2.15(2)	2(2)					
1Imd	1.99(2)	2(1)	neg2(2)	0.0703	318.571	29.503	9
1N/O	2.13(2)	2(2)					
1S	0	26(25)					
1Imd	1.95(4)	4(4)					
1Imd	2.06(4)	6(5)					
1Imd	2.18(4)	5(4)	neg3(2)	0.0778	352.758	40.096	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)					
1Br	2.42(5)	15(6)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1253	568.211	44.399	7
2N/O	2.13(2)	2(2)					
1Br	2.41(5)	17(7)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	1(2)	neg1(2)	0.0727	329.394	30.505	9
1N/O	2.14(2)	2(2)	neg1(2)	0.0852	386.091	43.885	11

1Br	2.41(5)	13(6)					
1Imd	1.98(3)	4(3)					
1Imd	2.11(4)	6(4)					
1Imd	2.23(4)	3(6)					

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)					
1Br	2.42(5)	16(7)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1256	569.299	44.484	7
2N/O	2.13(2)	2(2)					
1Br	2.42(5)	17(7)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	1(2)	neg1(2)	0.0723	327.615	30.341	9
1N/O	2.14(2)	2(2)					
1Br	2.41(5)	14(6)					
1Imd	2.23(4)	3(5)					
1Imd	2.11(4)	6(4)					
1Imd	1.98(3)	4(3)	neg1(2)	0.0847	383.911	43.637	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)					
1Br	2.42(5)	16(7)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1256	569.575	44.506	7
2N/O	2.13(2)	2(2)					
1Br	2.42(5)	18(7)					
1Imd	2.16(2)	1(2)					
1Imd	2.00(2)	2(1)	neg1(2)	0.0718	325.390	30.135	9
1N/O	2.14(2)	2(2)					
1Br	2.41(5)	14(6)					
1Imd	2.11(4)	6(4)					
1Imd	1.98(3)	5(3)					
1Imd	2.23(4)	4(5)	neg1(2)	0.0841	381.105	43.318	11

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(2)	2(1)					
1Br	2.42(5)	16(7)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1256	569.372	44.490	7
2N/O	2.13(2)	2(2)					
1Br	2.42(5)	18(7)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	1(2)	neg1(2)	0.0713	323.384	29.949	9

1N/O	2.14(2)	2(2)					
1Br	2.78(5)	13(6)					
1Imd	2.20(3)	5(4)					
1Imd	1.97(3)	5(3)					
1Imd	2.08(3)	7(4)	neg2(2)	0.0802	363.689	41.338	11

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(9)	12(11)					
2S	2.26(2)	6(1)					
1Imd	1.96(3)	3(3)	neg12(4)	0.1035	469.403	36.678	7
1N/O	1.97(6)	3(6)					
2S	2.25(2)	4(1)					
1Imd	1.95(4)	2(3)					
1Imd	1.78(6)	9(8)	neg16(3)	0.0921	417.696	38.683	9
0N/O							
2S	2.28(2)	6(2)					
1Imd	1.95(4)	4(3)					
1Imd	1.84(6)	4(7)					
1Imd	2.09(5)	3(3)	neg12(3)	0.1033	468.303	43.370	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(9)	12(11)					
2S	2.26(2)	6(1)					
1Imd	1.95(3)	3(3)	neg13(4)	0.1085	491.760	38.425	7
1N/O	1.96(6)	3(6)					
2S	2.25(2)	4(1)					
1Imd	1.95(4)	2(3)					
1Imd	1.77(5)	9(7)	neg17(3)	0.0948	429.809	39.805	9
0N/O							
2S	2.27(2)	6(2)					
1Imd	1.95(4)	4(3)					
1Imd	1.83(6)	3(7)					
1Imd	2.08(5)	3(4)	neg13(4)	0.1092	494.869	45.830	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(0.10)	13(12)					
2S	2.26(2)	6(1)					
1Imd	1.95(3)	3(3)	neg14(4)	0.1118	506.929	39.610	7
1N/O	2.13(2)	2(2)					
2S	2.35(5)	20(7)	neg4(3)	0.0950	430.671	39.885	9

1Imd	1.98(2)	2(1)					
1Imd	2.13(3)	1(3)					
0N/O							
2S	2.27(2)	6(2)					
1Imd	1.94(4)	4(3)					
1Imd	1.82(6)	3(7)					
1Imd	2.07(5)	3(4)	neg14(4)	0.1130	512.408	47.455	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(0.12)	16(14)					
2S	2.26(2)	6(1)					
1Imd	1.95(3)	3(3)	neg15(4)	0.1142	517.742	40.455	7
1N/O	2.13(2)	2(2)					
2S	2.37(6)	23(9)					
1Imd	2.13(3)	2(3)					
1Imd	1.99(2)	3(1)	neg4(3)	0.0973	441.261	40.866	9
0N/O							
2S	2.24(3)	5(1)					
1Imd	1.94(3)	1(3)					
1Imd	1.72(0.15)	10(13)					
1Imd	1.45(9)	10(12)	neg19(5)	0.1169	529.792	49.065	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(0.17)	20(16)					
2S	2.25(2)	5(1)					
1Imd	1.95(2)	2(2)	neg17(5)	0.1156	523.892	40.936	7
1N/O	2.13(2)	2(2)					
2S	2.39(7)	26(10)					
1Imd	2.14(3)	2(2)					
1Imd	1.99(2)	3(1)	neg3(2)	0.0988	447.995	41.489	9
0N/O							
2S	2.26(2)	6(2)					
1Imd	1.93(4)	3(4)					
1Imd	1.80(7)	4(7)					
1Imd	2.06(6)	2(5)	neg16(4)	0.1168	529.611	49.048	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	1(1)					
2Br	2.46(7)	23(10)					
1Imd	2.02(3)	1(2)	neg1(3)	0.1767	800.853	62.577	7

1N/O	2.14(3)	1(3)					
2Br	2.45(7)	24(10)					
1Imd	2.01(2)	2(1)					
1Imd	2.16(3)	2(2)	neg1(3)	0.1331	603.600	55.900	9
0N/O							
2Br	2.43(5)	17(7)					
1Imd	2.22(7)	4(11)					
1Imd	2.12(6)	6(8)					
1Imd	2.00(4)	5(5)	neg1(3)	0.2165	981.406	90.889	11

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	1(1)					
2Br	2.46(7)	23(10)					
1Imd	2.02(3)	1(2)	neg1(3)	0.1768	801.595	62.635	7
1N/O	2.14(3)	1(3)					
2Br	2.45(7)	24(10)					
1Imd	2.16(3)	2(2)					
1Imd	2.01(2)	2(1)	neg1(2)	0.1328	601.913	55.744	9
0N/O							
2Br	2.43(5)	17(7)					
1Imd	2.22(6)	4(10)					
1Imd	2.12(6)	6(7)					
1Imd	2.00(4)	5(5)	neg1(3)	0.2163	980.395	90.795	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(2)	2(1)					
2Br	2.52(9)	25(13)					
1Imd	1.61(5)	13(7)	neg7(3)	0.1912	866.818	67.732	7
1N/O	2.14(3)	1(3)					
2Br	2.45(7)	24(10)					
1Imd	2.01(2)	2(1)					
1Imd	2.16(3)	2(2)	neg1(2)	0.1320	598.504	55.428	9

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(2)	1(1)					
2Br	2.46(7)	24(10)					
1Imd	2.02(3)	1(2)	neg1(3)	0.1763	799.122	62.442	7
1N/O	2.14(3)	1(3)					
2Br	2.45(7)	24(10)					
1Imd	2.01(2)	2(1)					
1Imd	2.16(3)	2(2)	neg1(2)	0.1313	595.181	55.120	9

Co-N(2.0) Co-S(2.2) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(4)	2(3)					
1S	2.28(2)	1(2)					
1Br	2.22(4)	7(5)					
1Imd	1.99(4)	5(4)	neg8(3)	0.0562	254.729	23.591	9
1N/O	2.09(2)	3(3)					
1S	2.35(3)	3(3)					
1Br	2.31(4)	3(4)					
1Imd	1.96(2)	2(2)					
1Imd	2.11(2)	2(2)	neg5(2)	0.0355	160.740	18.270	11
1N/O	2.02(4)	3(5)					
2S	2.33(3)	1(2)					
1Br	2.31(3)	3(2)					
1Imd	1.98(4)	4(4)	neg8(2)	0.0489	221.825	20.543	9
1N/O	2.00(4)	1(4)					
1S	2.26(2)	1(2)					
2Br	2.16(6)	17(10)					
1Imd	1.98(5)	3(4)	neg10(3)	0.0882	399.624	37.010	9

Co-N(2.0) Co-S(2.2) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(4)	2(3)					
1S	2.29(2)	1(2)					
1Br	2.23(4)	8(5)					
1Imd	1.99(4)	5(4)	neg8(3)	0.0544	246.475	22.826	9
1N/O	2.09(2)	3(3)					
1S	2.34(3)	2(3)					
1Br	2.31(4)	4(4)					
1Imd	1.96(2)	2(1)					
1Imd	2.11(2)	2(2)	neg5(2)	0.0342	154.978	17.615	11
1N/O	1.42(0.11)	21(16)					
2S	2.30(3)	1(2)					
1Br	2.28(4)	4(3)					
1Imd	2.00(2)	2(1)	neg9(3)	0.0741	336.017	31.119	9
1N/O	2.01(4)	1(4)					
1S	2.26(2)	1(2)					
2Br	2.17(6)	17(8)					
1Imd	1.98(4)	3(4)	neg10(3)	0.0832	376.965	34.911	9

Co-N(2.0) Co-S(2.4) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2N/O	2.06(4)	1(3)					
1S	2.29(2)	2(2)					
1Br	2.22(4)	6(5)					
1Imd	1.98(5)	4(5)	neg9(3)	0.0607	275.329	25.498	9
1N/O	2.10(2)	3(3)					
1S	2.36(4)	3(4)					
1Br	2.31(5)	2(4)					
1Imd	2.11(2)	2(2)					
1Imd	1.95(3)	3(2)	neg6(2)	0.0361	163.759	18.614	11
1N/O	2.02(4)	2(5)					
2S	2.34(3)	1(2)					
1Br	2.32(3)	2(2)					
1Imd	1.98(4)	4(3)	neg9(2)	0.0469	212.626	19.692	9
1N/O	2.00(4)	1(5)					
1S	2.26(3)	1(2)					
2Br	2.15(7)	17(11)					
1Imd	1.97(5)	3(5)	neg11(3)	0.0937	424.916	39.352	9

Co-N(2.0) Co-S(2.4) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(4)	2(3)					
1S	2.29(2)	1(2)					
1Br	2.23(4)	7(5)					
1Imd	1.98(4)	4(4)	neg9(3)	0.0582	264.020	24.451	9
1N/O	2.10(2)	3(3)					
1S	2.35(3)	3(3)					
1Br	2.32(4)	3(4)					
1Imd	1.95(2)	3(1)					
1Imd	2.11(2)	2(2)	neg6(2)	0.0347	157.309	17.880	11
1N/O	2.03(4)	3(5)					
2S	2.33(3)	2(2)					
1Br	2.31(3)	3(2)					
1Imd	1.98(4)	4(3)	neg9(2)	0.0473	214.239	19.841	9
1N/O	2.01(4)	1(4)					
1S	2.26(2)	1(2)					
2Br	2.17(6)	17(9)					
1Imd	1.97(5)	3(5)	neg11(3)	0.0880	398.883	36.941	9

Co-N(2.0) Co-S(2.6) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(4)	1(3)					
1S	2.28(2)	1(2)					
1Br	2.22(5)	6(5)					
1Imd	1.97(5)	4(5)	neg9(3)	0.0648	293.712	27.201	9

1N/O	2.1(3)	1(2)					
1S	2.40(5)	2(5)					
1Br	2.36(5)	1(4)					
1Imd	1.96(2)	2(1)					
1Imd	2.12(2)	1(2)	neg5(2)	0.0684	174.238	19.805	11
1N/O	2.02(4)	2(4)					
2S	2.35(3)	2(3)					
1Br	2.32(3)	2(2)					
1Imd	1.97(4)	4(3)	neg10(2)	0.0476	215.760	19.982	9
1N/O	2.00(5)	1(4)					
1S	2.26(3)	1(2)					
2Br	2.15(7)	17(11)					
1Imd	1.96(5)	4(5)	neg12(4)	0.0962	436.265	40.403	9

Co-N(2.0) Co-S(2.6) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(4)	1(3)					
1S	2.29(2)	1(2)					
1Br	2.23(5)	7(5)					
1Imd	1.97(5)	4(4)	neg9(3)	0.0619	280.509	25.978	9
1N/O	2.10(2)	1(3)					
1S	2.38(4)	2(4)					
1Br	2.34(5)	3(4)					
1Imd	2.11(2)	1(2)					
1Imd	1.96(2)	3(1)	neg5(2)	0.0375	170.133	19.338	11
1N/O	2.02(4)	3(5)					
2S	2.34(3)	2(3)					
1Br	2.32(3)	3(2)					
1Imd	1.97(3)	4(3)	neg10(2)	0.0478	216.765	20.075	9
1N/O	2.00(4)	2(4)					
1S	2.26(3)	1(2)					
2Br	2.16(6)	16(9)					
1Imd	1.96(5)	3(5)	neg12(3)	0.0902	408.961	37.874	9

Co-N(2.0) Co-S(2.3) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.09(5)	13(5)					
1S	2.28(12)	3(1)					
1Imd	1.99(3)	4(2)	neg8(3)	0.0757	343.000	26.801	7
3N/O	2.14(2)	4(2)					
1S	2.26(5)	15(12)					
1Imd	2.14(3)	1(2)					
1Imd	1.98(2)	1(1)	neg3(2)	0.0584	264.877	24.531	9

2N/O	2.12(2)	2(2)					
1S	2.37(0.13)	28(35)					
1Imd	2.03(8)	2(7)					
1Imd	2.17(4)	3(4)					
1Imd	1.95(9)	1(12)	neg4(3)	0.0573	259.813	29.531	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(5)	13(5)					
1S	2.28(1)	3(1)					
1Imd	1.98(3)	4(3)	neg8(3)	0.0789	357.802	27.958	7
3N/O	2.13(2)	4(2)					
1S	2.27(6)	18(14)					
1Imd	1.98(2)	1(1)					
1Imd	2.14(3)	1(2)	neg3(2)	0.0603	273.562	25.335	9
2N/O	2.12(2)	2(2)					
1S	2.40(0.16)	31(38)					
1Imd	1.95(8)	1(11)					
1Imd	2.17(4)	3(4)					
1Imd	2.03(7)	2(7)	neg3(3)	0.0572	259.360	29.480	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(5)	13(5)					
1S	2.28(1)	3(1)					
1Imd	1.98(3)	4(3)	neg8(3)	0.0819	371.163	29.002	7
3N/O	2.12(2)	5(2)					
1S	2.65(7)	20(11)					
1Imd	2.00(2)	1(1)					
1Imd	2.16(2)	1(1)	neg1(1)	0.0571	258.891	23.976	9
2N/O	2.12(2)	2(2)					
1S	2.42(0.17)	33(39)					
1Imd	2.17(4)	3(4)					
1Imd	1.95(8)	1(10)					
1Imd	2.03(6)	2(8)	neg3(2)	0.0570	258.405	29.371	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(2)	7(3)					
1S	2.71(7)	16(11)					
1Imd	2.12(0.11)	10(13)	1(2)	0.1332	604.007	47.196	7
3N/O	2.12(2)	5(2)					
1S	2.65(7)	20(12)	neg1(1)	0.0569	258.112	23.904	9

1Imd	2.00(2)	1(1)					
1Imd	2.16(2)	1(1)					
2N/O	2.12(2)	2(2)					
1S	2.43(0.17)	34(39)					
1Imd	2.03(6)	3(7)					
1Imd	1.95(7)	1(10)					
1Imd	2.17(4)	3(4)	neg3(2)	0.0568	257.417	29.259	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.14(2)	4(1)					
1Br	2.40(4)	14(5)					
1Imd	1.99(2)	1(2)	neg1(2)	0.1049	475.412	37.148	7
3N/O	2.13(2)	5(2)					
1Br	2.40(4)	16(5)					
1Imd	1.99(2)	1(1)					
1Imd	2.16(2)	1(2)	neg1(1)	0.0497	225.357	20.871	9
2N/O	2.14(2)	2(2)					
1Br	2.41(4)	13(4)					
1Imd	1.99(3)	3(3)					
1Imd	2.24(7)	1(9)					
1Imd	2.12(5)	3(5)	neg1(2)	0.0521	236.134	26.843	11

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(3)	9(3)					
1Br	2.42(2)	11(3)					
1Imd	2.12(9)	9(12)	1(2)	0.1118	506.913	39.609	7
3N/O	2.13(2)	5(2)					
1Br	2.40(4)	16(5)					
1Imd	2.16(2)	1(2)					
1Imd	1.99(2)	1(1)	neg1(1)	0.0496	224.640	20.804	9
2N/O	2.14(2)	2(2)					
1Br	2.41(4)	13(5)					
1Imd	1.99(3)	3(3)					
1Imd	2.12(5)	3(5)					
1Imd	2.24(7)	1(9)	neg1(2)	0.0520	235.837	26.806	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(3)	9(3)					
1Br	2.43(3)	12(3)					
1Imd	2.12(9)	9(12)	1(2)	0.1123	509.075	39.778	7

3N/O	2.13(2)	5(2)					
1Br	2.40(4)	16(5)					
1Imd	2.16(2)	1(2)					
1Imd	1.99(2)	1(1)	neg1(1)	0.0493	223.628	20.710	9
2N/O	2.14(2)	2(2)					
1Br	2.41(4)	13(5)					
1Imd	2.12(5)	3(5)					
1Imd	2.24(7)	1(9)					
1Imd	1.99(3)	3(3)	neg1(2)	0.0518	235.026	26.714	11

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(1)	3(1)					
1Br	3.03(3)	10(4)					
1Imd	1.97(2)	1(1)	neg2(2)	0.1071	485.416	37.930	7
3N/O	2.13(2)	5(2)					
1Br	2.40(4)	16(5)					
1Imd	1.99(2)	1(1)					
1Imd	2.16(2)	1(2)	neg1(1)	0.0491	222.727	20.627	9
2N/O	2.13(2)	2(2)					
1Br	2.79(7)	17(9)					
1Imd	2.06(8)	1(25)					
1Imd	1.97(0.14)	1(13)					
1Imd	2.18(6)	2(9)	neg2(2)	0.0570	258.242	29.353	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(8)	16(12)					
2S	2.26(2)	6(2)					
1Imd	1.96(3)	3(2)	neg13(4)	0.1051	476.319	37.219	7
2N/O	1.98(6)	8(7)					
2S	2.25(2)	5(1)					
1Imd	1.76(5)	7(5)					
1Imd	1.94(3)	2(3)	neg16(3)	0.0868	393.413	36.434	9
1N/O	2.13(2)	1(2)					
2S	2.39(8)	27(15)					
1Imd	2.05(5)	5(6)					
1Imd	2.17(4)	4(4)					
1Imd	1.94(4)	2(6)	neg4(3)	0.0695	315.138	35.820	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(8)	17(13)					
2S	2.26(2)	6(2)	neg13(4)	0.1090	493.936	38.595	7

1Imd	1.96(3)	3(2)					
2N/O	2.13(2)	2(2)					
2S	2.45(0.13)	40(21)					
1Imd	1.99(2)	2(1)					
1Imd	2.15(2)	1(2)	neg2(2)	0.0659	298.884	27.680	9
1N/O	2.13(2)	2(2)					
2S	2.41(9)	29(17)					
1Imd	2.05(4)	5(5)					
1Imd	1.94(4)	3(5)					
1Imd	2.17(4)	4(4)	neg4(2)	0.0697	315.916	35.908	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	3(2)					
2S	2.28(3)	15(7)					
1Imd	1.97(2)	1(2)	neg7(4)	0.1113	504.533	39.423	7
2N/O	2.13(2)	2(2)					
2S	2.47(0.13)	41(21)					
1Imd	2.15(2)	2(2)					
1Imd	1.99(2)	2(1)	neg2(2)	0.0659	298.622	27.656	9
1N/O	2.13(2)	2(2)					
2S	2.42(9)	31(17)					
1Imd	1.94(4)	3(5)					
1Imd	2.05(4)	5(5)					
1Imd	2.18(4)	5(3)	neg4(2)	0.0696	315.465	35.857	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	3(2)					
2S	2.28(4)	15(7)					
1Imd	1.97(2)	1(2)	neg7(4)	0.1138	515.725	40.298	7
2N/O	2.13(2)	2(2)					
2S	2.48(0.13)	42(22)					
1Imd	1.99(2)	2(1)					
1Imd	2.15(2)	2(2)	neg2(2)	0.0658	298.453	27.640	9
1N/O	2.13(2)	2(2)					
2S	2.43(9)	32(17)					
1Imd	1.94(3)	3(4)					
1Imd	2.05(4)	6(4)					
1Imd	2.18(3)	5(3)	neg4(2)	0.0694	314.657	35.765	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)	neg1(2)	0.1286	583.173	45.568	7

2Br	2.43(6)	23(9)					
1Imd	2.00(2)	1(2)					
2N/O	2.13(2)	2(2)					
2Br	2.41(6)	25(10)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	1(2)	neg1(2)	0.0758	343.782	31.838	9
1N/O	2.14(2)	2(2)					
2Br	2.40(6)	21(8)					
1Imd	1.98(3)	5(3)					
1Imd	2.23(4)	4(5)					
1Imd	2.10(4)	6(5)	neg1(2)	0.0913	414.078	47.066	11

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)					
2Br	2.43(6)	24(9)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1289	584.203	45.649	7
2N/O	2.13(2)	2(2)					
2Br	2.41(6)	26(10)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	2(2)	neg1(2)	0.0753	341.363	31.614	9
1N/O	2.14(2)	2(2)					
2Br	2.40(6)	22(9)					
1Imd	1.98(3)	5(3)					
1Imd	2.10(4)	6(4)					
1Imd	2.22(4)	4(5)	neg1(2)	0.0906	410.528	46.662	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)					
2Br	2.44(7)	24(10)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1289	584.214	45.649	7
2N/O	2.13(2)	2(2)					
2Br	2.42(6)	26(10)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	2(2)	neg1(2)	0.0747	338.485	31.347	9
1N/O	2.14(2)	2(2)					
2Br	2.40(6)	22(9)					
1Imd	2.10(4)	6(4)					
1Imd	1.98(3)	5(3)					
1Imd	2.22(4)	4(5)	neg1(2)	0.0896	406.405	46.194	11

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)					
2Br	2.44(7)	24(10)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1288	583.877	45.623	7
2N/O	2.13(2)	2(2)					
2Br	2.42(6)	26(9)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	2(2)	neg1(2)	0.0741	336.119	31.128	9
1N/O	2.14(2)	2(2)					
2Br	2.40(6)	22(9)					
1Imd	2.10(4)	6(4)					
1Imd	2.22(4)	4(5)					
1Imd	1.98(3)	5(3)	neg1(2)	0.0890	403.343	45.846	11

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.13(2)	3(2)					
2S	2.26(3)	13(6)					
1Imd	1.97(2)	1(2)	neg7(3)	0.0993	450.180	35.176	7
2N/O	2.13(2)	2(2)					
2S	2.41(0.15)	40(23)					
1Imd	2.14(2)	1(2)					
1Imd	1.99(1)	2(1)	neg3(2)	0.0571	258.828	23.970	9
1N/O	2.13(2)	1(2)					
2S	2.37(7)	26(15)					
1Imd	2.04(6)	4(6)					
1Imd	2.17(4)	3(4)					
1Imd	1.95(6)	1(9)	neg4(3)	0.0628	284.601	32.349	11

Co-N(2.2) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.15(2)	2(1)					
2S	2.44(7)	24(10)					
1Imd	2.00(2)	1(2)	neg1(2)	0.1288	583.877	45.623	7
2N/O	2.13(2)	2(2)					
2S	2.42(6)	26(9)					
1Imd	2.00(2)	2(1)					
1Imd	2.16(2)	2(2)	neg1(2)	0.0741	336.119	31.128	9
1N/O	2.14(2)	2(2)					
2S	2.40(6)	22(9)					
1Imd	2.10(4)	6(4)					
1Imd	2.22(4)	4(5)					
1Imd	1.98(3)	5(3)	neg1(2)	0.0890	403.343	45.846	11

Co-N(2.0) Co-N(2.2) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(2)	4(2)					
1N/O	2.17(1)	5(1)					
2S	2.40(9)	32(16)					
1Imd	1.96(5)	2(5)					
1Imd	2.10(5)	1(4)	neg4(3)	0.0319	144.540	16.429	11

Co-N(2.0) Co-S(2.2) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(3)	9(4)					
1S	2.50(3)	7(3)					
1S	2.30(1)	1(1)					
1Imd	2.01(3)	5(3)	neg6(2)	0.0400	181.501	16.809	9
2N/O	2.09(3)	5(3)					
1S	2.53(3)	6(3)					
1S	2.32(2)	3(2)					
1Imd	1.97(2)	0(2)					
1Imd	2.12(3)	1(2)	neg5(2)	0.0254	115.314	13.107	11
1N/O	2.86(5)	3(5)					
1S	2.30(2)	3(1)					
1S	1.77(4)	19(5)					
1Imd	2.16(3)	6(2)					
1Imd	2.02(3)	4(2)					
1Imd	2.31(4)	2(3)	neg1(2)	0.0343	155.314	22.847	13

Co-N(2.0) Co-S(2.2) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	6(3)					
1S	2.31(2)	3(2)					
1S	2.54(3)	8(3)					
1Imd	1.97(2)	0(2)					
1Imd	2.12(2)	1(2)	neg5(1)	0.0234	105.916	12.039	11

Co-N(2.0) Co-S(2.2) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	6(3)					
1S	2.31(2)	3(2)					
1S	2.54(3)	9(3)					
1Imd	1.97(2)	0(2)					
1Imd	2.12(2)	1(2)	neg5(1)	0.0225	101.853	11.577	11

Co-N(2.0) Co-S(2.2) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	7(3)					
1S	2.30(2)	3(2)	neg5(1)	0.0217	98.592	11.206	11

1S	2.54(3)	9(3)					
1Imd	1.97(2)	0(1)					
1Imd	2.12(2)	1(2)					

Co-N(2.0) Co-S(2.3) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	6(3)					
1S	2.31(2)	3(2)					
1S	2.54(3)	7(3)					
1Imd	2.12(2)	1(2)					
1Imd	1.97(2)	0(2)	neg5(2)	0.0237	107.596	12.230	11

Co-N(2.0) Co-S(2.3) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	6(3)					
1S	2.31(2)	3(2)					
1S	2.54(3)	8(3)					
1Imd	2.12(2)	1(2)					
1Imd	1.97(2)	0(1)	neg5(1)	0.0228	103.385	11.751	11

Co-N(2.0) Co-S(2.3) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	6(3)					
1S	2.31(2)	3(2)					
1S	2.55(3)	8(3)					
1Imd	2.12(2)	1(2)					
1Imd	1.97(2)	0(1)	neg5(1)	0.0221	100.026	11.369	11

Co-N(2.0) Co-S(2.4) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	5(3)					
1S	2.32(2)	3(2)					
1S	2.55(3)	7(3)					
1Imd	2.12(2)	1(2)					
1Imd	1.97(2)	1(1)	neg5(1)	0.0232	105.053	11.941	11

Co-N(2.0) Co-S(2.4) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	6(3)					
1S	2.31(2)	3(2)					
1S	2.55(3)	8(3)					
1Imd	2.12(2)	1(2)					
1Imd	1.97(2)	1(1)	neg5(1)	0.0224	101.588	11.547	11

Co-N(2.0) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(3)	5(3)					
1S	2.55(3)	7(3)	neg5(2)	0.0248	112.489	12.786	11

1S	2.32(2)	4(2)					
1Imd	1.97(2)	1(1)					
1Imd	2.12(2)	1(2)					

Co-N(2.0) Co-S(2.2) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	4(3)					
1S	2.36(4)	1(4)					
1Br	2.33(5)	6(3)					
1Imd	2.12(3)	1(2)					
1Imd	1.97(2)	1(1)	neg4(2)	0.0283	128.439	14.599	11

Co-N(2.0) Co-S(2.2) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	4(3)					
1S	2.35(4)	1(3)					
1Br	2.33(4)	6(3)					
1Imd	1.97(2)	1(1)					
1Imd	2.12(3)	0(2)	neg4(2)	0.0280	126.835	14.417	11

Co-N(2.0) Co-S(2.2) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	4(3)					
1S	2.35(4)	1(3)					
1Br	2.33(4)	7(3)					
1Imd	2.12(3)	0(2)					
1Imd	1.97(2)	1(1)	neg5(2)	0.0276	124.904	14.197	11

Co-N(2.0) Co-S(2.2) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(3)	3(3)					
1S	2.31(4)	9(6)					
1Br	2.74(5)	13(5)					
1Imd	2.12(3)	1(3)					
1Imd	1.97(2)	2(1)	neg4(2)	0.0527	239.089	27.176	11

Co-N(2.0) Co-S(2.3) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(3)					
1S	2.37(5)	1(5)					
1Br	2.35(5)	5(3)					
1Imd	1.97(2)	1(1)					
1Imd	2.13(3)	1(2)	neg4(2)	0.0281	127.269	14.466	11

Co-N(2.0) Co-S(2.3) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	4(3)					
1S	2.36(4)	1(4)	neg4(2)	0.0279	126.426	14.370	11

1Br	2.34(5)	5(3)					
1Imd	2.12(3)	1(2)					
1Imd	1.97(2)	1(1)					

Co-N(2.0) Co-S(2.3) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	4(3)					
1S	2.36(4)	1(4)					
1Br	2.34(4)	6(3)					
1Imd	1.97(2)	1(1)					
1Imd	2.12(3)	1(2)	neg5(2)	0.0275	124.662	14.170	11

Co-N(2.0) Co-S(2.3) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(2)	2(2)					
1S	2.31(4)	10(7)					
1Br	2.74(5)	13(4)					
1Imd	2.11(3)	1(3)					
1Imd	1.97(2)	2(1)	neg4(2)	0.0545	247.205	28.098	11

Co-N(2.0) Co-S(2.4) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(3)	5(3)					
1S	2.39(5)	1(5)					
1Br	2.36(5)	4(4)					
1Imd	2.13(3)	1(2)					
1Imd	1.97(2)	1(1)	neg4(2)	0.0281	127.212	14.459	11

Co-N(2.0) Co-S(2.4) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(3)					
1S	2.38(5)	1(5)					
1Br	2.35(5)	5(3)					
1Imd	1.97(2)	1(1)					
1Imd	2.12(3)	1(2)	neg4(2)	0.0280	127.056	14.442	11

Co-N(2.0) Co-S(2.4) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(3)					
1S	2.37(4)	1(4)					
1Br	2.35(5)	6(3)					
1Imd	2.12(3)	1(2)					
1Imd	1.97(2)	1(1)	neg5(2)	0.0277	125.510	14.266	11

Co-N(2.0) Co-S(2.4) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(2)	2(2)					
1S	2.32(4)	11(7)	neg4(2)	0.0560	254.006	28.871	11

1Br	2.74(5)	12(4)					
1Imd	1.97(2)	2(1)					
1Imd	2.11(3)	1(3)					

Co-N(2.0) Co-S(2.5) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(3)	5(3)					
1S	2.40(5)	1(6)					
1Br	2.37(5)	4(4)					
1Imd	1.97(2)	1(1)					
1Imd	2.13(2)	1(2)	neg4(2)	0.0280	127.057	14.442	11

Co-N(2.0) Co-S(2.5) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(3)					
1S	2.39(5)	2(5)					
1Br	2.36(5)	5(4)					
1Imd	2.13(2)	1(2)					
1Imd	1.97(2)	1(1)	neg4(2)	0.0282	127.898	14.537	11

Co-N(2.0) Co-S(2.5) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(3)					
1S	2.39(5)	2(5)					
1Br	2.36(5)	5(3)					
1Imd	1.97(2)	1(1)					
1Imd	2.12(2)	1(2)	neg4(2)	0.0280	127.001	14.435	11

Co-N(2.0) Co-S(2.5) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(2)	2(2)					
1S	2.32(4)	12(8)					
1Br	2.75(5)	12(4)					
1Imd	2.11(3)	1(3)					
1Imd	1.97(2)	2(1)	neg4(2)	0.0574	260.139	29.568	11

Co-N(2.0) Co-S(2.6) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(3)	5(3)					
1S	2.41(5)	1(6)					
1Br	2.37(4)	4(4)					
1Imd	1.97(2)	1(1)					
1Imd	2.13(2)	1(2)	neg4(2)	0.0278	126.079	14.331	11

Co-N(2.0) Co-S(2.6) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(2)	5(3)					
1S	2.40(5)	2(6)	neg4(2)	0.0282	127.750	14.521	11

1Br	2.37(4)	5(4)					
1Imd	1.97(2)	1(1)					
1Imd	2.13(2)	1(2)					

Co-N(2.0) Co-S(2.6) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(2)	5(2)					
1S	2.40(5)	2(5)					
1Br	2.37(4)	5(3)					
1Imd	2.13(2)	1(2)					
1Imd	1.97(2)	1(1)	neg4(2)	0.0281	127.465	14.488	11

Co-N(2.0) Co-S(2.6) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(2)					
1S	2.39(5)	3(5)					
1Br	2.37(4)	5(3)					
1Imd	1.97(2)	1(1)					
1Imd	2.13(2)	1(2)	neg4(2)	0.0278	125.961	14.317	11

Co-N(2.0) Co-N(2.2) Co-S(2.3) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	1(3)					
1N/O	2.14(2)	4(2)					
1S	2.37(4)	6(5)					
1S	2.61(4)	7(4)					
1Imd	2.17(4)	2(4)					
1Imd	2.02(3)	1(3)	neg3(2)	0.0175	79.396	11.680	11

Co-N(2.0) Co-N(2.2) Co-S(2.3) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	1(3)					
1N/O	2.14(2)	4(2)					
1S	2.36(4)	7(4)					
1S	2.61(4)	8(4)					
1Imd	2.17(4)	1(3)					
1Imd	2.01(3)	1(2)	neg3(1)	0.0153	69.320	10.197	11

Co-N(2.0) Co-N(2.2) Co-S(2.2) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	1(3)					
1N/O	2.14(2)	4(2)					
1S	2.35(4)	7(4)					
1S	2.61(4)	9(4)					
1Imd	2.02(3)	1(3)					
1Imd	2.17(4)	2(4)	neg3(1)	0.0156	70.802	10.415	11

Table F.11. Additional Fits for Zn(II) E34C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(3)	1(2)	14(6)	0.3915	15920.836	2342.376	3
3N/O	2.15(3)	3(2)	12(5)	0.3407	13855.425	2038.499	3
4N/O	2.14(3)	5(3)	10(4)	0.3345	13602.504	2001.288	3
5N/O	2.13(4)	7(3)	8(4)	0.3553	14448.939	2125.821	3
6N/O	2.12(4)	8(3)	6(5)	0.3894	15835.190	2329.775	3
7N/O	2.10(5)	10(4)	4(5)	0.4284	17424.827	2563.653	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.27(2)	4(1)	neg2(5)	0.1689	6868.436	1010.529	3
3S	2.26(2)	6(1)	neg4(4)	0.1384	5630.332	828.371	3
4S	2.25(2)	9(1)	neg6(4)	0.1485	6041.557	888.873	3
5S	2.25(3)	11(2)	neg8(4)	0.1768	7188.884	1057.675	3
6S	2.24(3)	13(2)	neg9(5)	0.2123	8635.521	1270.513	3
7S	2.23(4)	14(2)	neg10(5)	0.2499	10162.451	1495.165	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.06(3)	2(2)					
1N/O	2.19(2)	6(2)	7(4)	0.1756	7140.198	1488.510	5
2N/O	2.03(3)	2(3)					
2N/O	2.17(2)	4(2)	6(4)	0.1998	8126.053	1694.031	5
3N/O	2.06(3)	1(3)					
1N/O	2.19(2)	6(2)	6(4)	0.1833	7453.861	1553.899	5
4N/O	2.06(3)	4(3)					
1N/O	2.18(3)	5(2)	4(4)	0.2154	8758.710	1825.920	5
3N/O	2.03(4)	2(3)					
2N/O	2.17(3)	3(2)	4(4)	0.2353	9567.895	1994.610	5
5N/O	2.06(4)	6(4)					
1N/O	2.18(3)	4(2)	3(4)	0.2582	10499.550	2188.831	5
4N/O	2.03(4)	4(4)					
2N/O	2.17(3)	2(3)	3(4)	0.2794	11364.038	2369.050	5
3N/O	2.00(4)	3(4)					
3N/O	2.15(3)	1(3)	2(4)	0.3013	12254.929	2554.774	5

6N/O	2.05(5)	9(5)					
1N/O	2.17(3)	4(3)	2(5)	0.3035	12342.339	2572.996	5
5N/O	2.03(5)	8(6)					
2N/O	2.16(4)	1(3)	1(5)	0.3236	13161.414	2743.748	5
4N/O	2.00(6)	6(6)					
3N/O	2.15(4)	1(3)	1(5)	0.3452	14040.766	2927.065	5

Zn-S(2.2) Zn-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(2)	3(2)					
1S	2.29(2)	2(1)	neg10(3)	0.0502	2041.105	425.507	5
2S	2.13(3)	4(2)					
2S	2.27(2)	1(1)	neg12(4)	0.0660	2683.302	559.385	5
3S	2.17(2)	7(2)					
1S	2.28(2)	1(1)	neg12(4)	0.0605	2461.431	513.132	5
4S	2.26(3)	9(2)					
1S	1.81(0.15)	29(34)	neg3(6)	0.1359	5526.343	1152.072	5
3S	2.14(3)	8(3)					
2S	2.27(2)	2(2)	neg13(4)	0.0903	3673.821	765.878	5
5S	2.24(2)	12(1)					
1S	2.59(1)	1(1)	neg10(3)	0.0231	939.795	195.918	5
4S	2.25(3)	5(2)					
2S	2.08(4)	6(4)	neg13(5)	0.1221	4967.589	1035.589	5
3S	2.11(4)	9(4)					
3S	2.25(3)	4(2)	neg14(5)	0.1256	5108.676	1065.001	5
6S	2.24(2)	14(1)					
1S	2.58(1)	1(1)	neg11(3)	0.0275	1118.858	233.247	5
5S	2.26(4)	11(2)					
2S	1.88(0.18)	38(41)	neg5(8)	0.1590	6468.324	1348.445	5
4S	2.24(3)	6(2)					
3S	2.09(5)	10(5)	neg15(5)	0.1477	6007.261	1252.328	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(3)	2(2)					5
1S	2.29(2)	1(1)	1(3)	0.0523	2128.655	443.759	

1N/O 2S	1.98(3) 2.27(2)	1(2) 3(1)	neg4(3)	0.0596	2424.147	505.360	5
2N/O 2S	1.99(4) 2.28(2)	4(3) 3(1)	neg3(4)	0.0789	3210.232	669.234	5
3N/O 1S	2.04(3) 2.30(2)	5(2) 1(1)	1(4)	0.0627	2549.675	531.528	5
1N/O 3S	1.95(4) 2.26(2)	1(3) 5(1)	neg6(4)	0.0964	3918.622	816.911	5
1N/O 4S	2.19(2) 2.21(2)	4(1) 6(1)	neg9(4)	0.0566	2303.829	480.277	5
4N/O 1S	2.05(5) 2.29(2)	9(3) 1(1)	1(5)	0.0830	3377.205	704.043	5
2N/O 3S	2.14(0.17) 2.27(3)	20(65) 7(3)	neg1(10)	0.1192	4847.193	1010.490	5
3N/O 2S	2.10(0.14) 2.28(3)	14(13) 5(2)	2(9)	0.0975	3967.403	827.081	5
5N/O 1S	2.07(8) 2.29(2)	13(5) 1(2)	1(6)	0.1037	4215.867	878.878	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.17(0.13) 2.29(3)	18(26) 4(2)	5(12)	0.0929	3778.705	787.743	5
2N/O 4S	2.20(2) 2.21(2)	3(1) 5(1)	neg8(4)	0.0509	2069.564	431.440	5
3N/O 3S	2.18(9) 2.28(3)	20(8) 7(3)	1(15)	0.1103	4485.176	935.020	5
6N/O 1S	2.09(0.11) 2.29(2)	17(6) 1(2)	2(8)	0.1218	4954.947	1032.953	5
1N/O 6S	2.43(2) 2.22(4)	4(1) 15(2)	neg13(5)	0.0772	3138.161	654.209	5
5N/O 2S	2.20(0.10) 2.29(2)	22(22) 4(1)	6(9)	0.0583	2371.858	494.459	5
2N/O	2.19(2)	2(1)	neg9(4)	0.0879	3573.488	744.962	5

5S	2.21(2)	7(1)					
4N/O	2.22(6)	17(37)					
3S	2.29(2)	7(2)	4(10)	0.0986	4011.054	836.181	5
3N/O	2.21(2)	2(1)					
4S	2.21(2)	4(1)	neg6(4)	0.0546	2219.493	462.696	5

Table F.12. Additional Fits for Zn(II) E34C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(2)	1(2)	14(4)	0.4267	19008.919	1131.628	3
3N/O	2.15(2)	3(2)	11(3)	0.3757	16179.618	963.196	3
4N/O	2.14(2)	5(2)	9(3)	0.3682	15853.800	943.799	3
5N/O	2.13(2)	7(2)	8(3)	0.3867	16652.917	991.372	3
6N/O	2.12(3)	9(2)	6(3)	0.4185	18019.556	1072.730	3
7N/O	2.10(3)	10(3)	4(3)	0.4555	19614.744	1167.694	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.27(2)	4(1)	neg2(4)	0.2040	8976.266	534.370	3
3S	2.26(2)	6(1)	neg4(3)	0.1790	7708.107	458.875	3
4S	2.25(2)	9(1)	neg6(3)	0.1884	8112.904	482.973	3
5S	2.25(2)	11(1)	neg7(3)	0.2151	9264.706	551.541	3
6S	2.24(2)	13(1)	neg9(3)	0.2490	10721.870	638.288	3
7S	2.23(3)	14(2)	neg10(4)	0.2848	12262.989	730.033	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.07(2)	2(2)					
1N/O	2.20(2)	6(1)	8(3)	0.2225	9581.358	647.483	5
2N/O	2.03(2)	1(2)					
2N/O	2.17(2)	3(1)	6(2)	0.2438	10498.989	709.494	5
3N/O	2.07(2)	1(2)					
1N/O	2.19(2)	5(1)	1(2)	0.2277	9805.888	662.656	5
4N/O	2.06(2)	4(2)					
1N/O	2.19(2)	5(1)	4(3)	0.2568	11057.733	747.253	5
3N/O	2.03(2)	2(2)					
2N/O	2.17(2)	2(1)	4(3)	0.2751	11846.324	800.544	5

5N/O	2.06(3)	6(2)					
1N/O	2.18(2)	4(2)	3(3)	0.2967	12778.241	863.520	5
4N/O	2.03(3)	5(3)					
2N/O	2.17(2)	2(2)	3(3)	0.3162	13618.304	920.289	5
3N/O	2.01(3)	3(3)					
3N/O	2.16(2)	1(2)	2(3)	0.3376	14538.461	982.471	5
6N/O	2.05(3)	9(3)					
1N/O	2.17(2)	3(2)	2(3)	0.3398	14630.399	988.384	5
5N/O	2.03(3)	7(3)					
2N/O	2.16(2)	1(2)	1(3)	0.3586	15441.543	1043.499	5
4N/O	2.00(3)	6(4)					
3N/O	2.15(2)	1(2)	1(3)	0.3797	16349.751	1104.873	5

Zn-S(2.2) Zn-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.17(2)	3(1)					
1S	2.29(1)	2(1)	neg10(3)	0.0928	3997.055	270.111	5
2S	2.13(2)	4(2)					
2S	2.27(1)	1(1)	neg12(3)	0.1079	4647.894	314.092	5
3S	2.17(2)	7(1)					
1S	2.29(1)	1(1)	neg12(3)	0.1027	4420.566	298.730	5
4S	2.26(2)	9(1)					
1S	1.81(0.10)	29(23)	neg3(4)	0.1763	7592.504	513.082	5
3S	2.14(2)	8(2)					
2S	2.27(2)	2(1)	neg13(3)	0.1314	5656.847	382.275	5
5S	2.25(3)	11(2)					
1S	1.89(0.22)	32(38)	neg6(5)	0.2048	8817.400	595.857	5
4S	2.25(2)	5(1)					
2S	2.09(3)	6(2)	neg13(3)	0.1630	7019.445	474.356	5
3S	2.11(3)	9(3)					
3S	2.26(2)	4(1)	neg14(3)	0.1659	7142.351	482.661	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.26(3)	11(2)	neg5(5)	0.1985	8546.637	577.559	5

2S	1.88(0.12)	38(27)					
4S	2.25(2)	6(2)					
3S	2.09(3)	10(3)	neg14(4)	0.1881	8101.596	547.485	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(2)	2(1)					5
1S	2.30(1)	1(1)	1(3)	0.0955	4112.397	277.905	
1N/O	1.98(2)	1(1)					5
2S	2.27(1)	3(1)	neg3(2)	0.1027	4424.130	298.971	
2N/O	2.00(3)	4(2)					
2S	2.28(1)	3(1)	neg3(3)	0.1201	5171.082	349.448	5
3N/O	2.04(2)	5(2)					
1S	2.30(1)	1(1)	1(3)	0.1050	4523.383	305.678	5
1N/O	1.96(3)	1(2)					
3S	2.26(2)	6(1)	neg6(3)	0.1375	5922.279	400.212	5
1N/O	2.20(2)	4(1)					
4S	2.22(2)	6(1)	neg8(3)	0.1022	4402.754	297.527	5
4N/O	2.05(3)	9(2)					
1S	2.29(1)	1(1)	1(3)	0.1249	5378.122	363.439	5
2N/O	2.13(0.12)	20(42)					
3S	2.27(2)	7(2)	neg1(6)	0.1610	6932.558	468.484	5
3N/O	2.08(9)	14(7)					
2S	2.28(2)	5(1)	1(5)	0.1402	6036.182	407.909	5
5N/O	2.07(5)	13(3)					
1S	2.29(2)	1(1)	1(4)	0.1455	6264.380	423.330	5
1N/O	2.76(3)	2(3)					
5S	2.24(2)	11(1)	neg8(3)	0.1742	7503.520	507.068	5
4N/O	2.16(9)	18(17)					
2S	2.29(2)	4(2)	4(8)	0.0963	4148.324	280.333	5
2N/O	2.20(2)	2(1)					
4S	2.22(2)	5(1)	neg7(3)	0.0963	4148.324	280.333	5
3N/O	2.18(7)	22(50)					
3S	2.28(2)	7(2)	1(9)	0.1534	6605.537	446.385	5

6N/O	2.09(7)	17(4)					
1S	2.29(2)	1(1)	2(5)	0.1637	7051.188	476.501	5
1N/O	2.43(1)	3(1)					
6S	2.22(3)	15(1)	neg13(4)	0.1183	5092.906	344.165	5
5N/O	2.19(7)	22(15)					
2S	2.29(2)	4(1)	6(6)	0.1334	5743.644	388.140	5
2N/O	2.19(2)	2(1)					
5S	2.21(2)	7(1)	neg9(3)	0.1036	4461.632	301.505	5
4N/O	2.21(5)	20(32)					
3S	2.28(2)	7(1)	3(8)	0.1442	6211.300	419.743	5
3N/O	2.21(2)	2(1)					
4S	2.22(2)	4(1)	neg6(3)	0.0998	4299.288	290.535	5

Zn-N(2.0) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(3)	2(2)					5
1Br	2.42(2)	4(1)	2(4)	0.1466	6529.744	441.263	
1N/O							5
2Br			No Fit	No Fit	No Fit	No Fit	
2N/O	2.00(3)	4(2)					
2Br	2.38(2)	7(1)	neg10(5)	0.1285	5533.190	373.918	5
3N/O	2.08(2)	4(1)					
1Br	2.42(1)	4(1)	2(3)	0.1053	4536.062	306.535	5
1N/O							
3Br			No Fit	No Fit	No Fit	No Fit	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.08(2)	7(1)					
1Br	2.42(1)	4(1)	2(3)	0.0929	3998.829	270.230	5
2N/O	1.95(3)	5(2)					
3Br	2.36(2)	9(1)	neg17(5)	0.1121	4828.735	326.313	5
3N/O	2.05(3)	6(2)					
2Br	2.41(2)	7(1)	neg2(4)	0.0992	4272.678	288.736	5
5N/O	2.16(2)	4(2)					
1Br	1.95(4)	11(5)	9(3)	0.3284	14142.960	955.744	5

1N/O 5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 2Br	2.06(2) 2.41(1)	8(2) 8(1)	neg1(3)	0.0854	3679.586	248.657	5
2N/O 4Br	1.93(3) 2.35(2)	6(2) 10(1)	neg20(4)	0.1064	4583.638	309.750	5
3N/O 3Br	1.98(3) 2.37(2)	8(2) 9(1)	neg12(5)	0.1019	4387.318	296.483	5
6N/O 1Br	2.02(3) 2.09(2)	6(2) 4(2)	neg1(3)	0.2667	11484.765	776.110	5
1N/O 6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O 2Br	2.06(3) 2.41(1)	11(2) 8(1)	neg2(3)	0.0841	3621.093	244.704	5
2N/O 5Br	1.91(3) 2.34(2)	6(3) 12(1)	neg22(4)	0.1069	4603.371	311.084	5
4N/O 3Br	2.04(3) 2.41(2)	10(2) 10(1)	neg3(4)	0.0926	3985.764	269.347	5
3N/O 4Br	1.94(4) 2.35(2)	9(3) 10(1)	neg18(5)	0.1022	4400.485	297.373	5

Zn-N(2.0) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O 1Imd	2.08(3) 2.18(3)	8(3) 1(3)	5(3)	0.3473	14955.499	1010.653	5
4N/O 1Imd 1Imd	2.06(5) 2.05(4) 2.18(3)	11(7) 3(4) 4(3)	3(3)	0.3002	12928.644	1010.220	7
3N/O 1Imd 1Imd 1Imd	2.08(5) 2.06(3) 2.18(3) 1.93(4)	7(6) 10(3) 9(2) 5(4)	1(3)	0.2431	10469.832	969.622	9
2N/O 1Imd 1Imd 1Imd	2.10(4) 2.06(3) 2.18(3) 1.94(3)	2(4) 15(3) 13(2) 14(3)	neg1(3)	0.1794	7723.793	877.918	11

1Imd	1.84(3)	7(5)					
1N/O	2.10(3)	3(4)					
1Imd	2.06(4)	19(5)					
1Imd	2.18(4)	16(4)					
1Imd	1.84(5)	13(8)					
1Imd	1.95(4)	18(6)					
1Imd	1.69(0.13)	6(23)	neg1(4)	0.0140	6025.529	886.387	13
4N/O	2.08(3)	6(3)					
1Imd	2.19(3)	1(2)	6(3)	0.3287	14156.537	956.662	5
3N/O	2.09(5)	7(6)					
1Imd	2.18(3)	3(2)					
1Imd	2.04(6)	0(5)	5(3)	0.2887	12430.563	971.301	7
2N/O	2.10(4)	3(5)					
1Imd	2.06(3)	10(2)					
1Imd	1.93(3)	7(3)					
1Imd	2.19(3)	10(2)	2(2)	0.2180	9387.211	869.359	9
1N/O	2.11(3)	2(3)					
1Imd	1.96(2)	16(3)					
1Imd	2.19(2)	14(2)					
1Imd	1.85(3)	10(4)					
1Imd	2.07(2)	17(2)	neg1(2)	0.1663	7160.741	813.919	11
0N/O							
1Imd	2.19(3)	15(3)					
1Imd	1.64(0.23)	17(35)					
1Imd	2.08(3)	17(4)					
1Imd	1.97(3)	16(5)					
1Imd	1.86(4)	10(7)	neg1(4)	0.2142	9222.595	1048.278	11
3N/O	2.14(3)	4(3)					
1Imd	2.10(0.14)	7(15)	8(4)	0.3622	15596.290	1053.956	5
2N/O	2.11(4)	3(5)					
1Imd	2.03(5)	1(4)					
1Imd	2.18(4)	3(2)	6(3)	0.2875	12378.602	967.241	7
1N/O	2.11(4)	2(4)					
1Imd	2.06(2)	11(2)					
1Imd	1.94(2)	8(2)					
1Imd	2.19(2)	10(2)	2(2)	0.2091	9003.696	833.841	9
0N/O							
1Imd	2.08(2)	17(3)					
1Imd	2.20(2)	15(2)					
1Imd	1.87(3)	10(4)	neg1(2)	0.2239	9642.236	892.977	9

1Imd	1.97(2)	16(3)					
2N/O	2.10(4)	2(4)					
1Imd	2.20(4)	2(3)	10(4)	0.3698	15924.596	1076.142	5
1N/O	2.14(4)	2(4)					
1Imd	2.03(3)	3(2)					
1Imd	2.17(4)	3(3)	7(3)	0.3145	13541.170	1058.082	7
0N/O							
1Imd	2.19(2)	11(2)					
1Imd	1.95(2)	9(2)					
1Imd	2.06(2)	12(2)	2(3)	0.2696	11611.669	907.314	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(4)	7(4)					
1S	2.29(1)	1(1)					
1Imd	2.05(3)	3(4)	neg1(2)	0.0802	3452.621	269.781	7
1N/O	2.01(2)	3(2)					
1S	2.28(1)	2(1)					
1Imd	2.05(3)	2(2)					
1Imd	1.89(3)	0(2)	neg5(2)	0.0480	2068.671	191.582	9
0N/O							
1S	2.28(1)	1(1)					
1Imd	1.94(2)	5(2)					
1Imd	2.19(3)	6(2)					
1Imd	2.06(2)	8(2)	1(2)	0.0562	2418.428	223.973	9

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(4)	6(4)					
1S	2.30(1)	0(1)					
1Imd	2.06(4)	3(4)	0(2)	0.0704	3136.057	245.046	7
1N/O	2.00(2)	4(1)					
1S	2.28(1)	2(1)					
1Imd	2.05(2)	2(1)					
1Imd	1.89(2)	1(2)	neg5(2)	0.0422	1818.475	168.133	9
0N/O							
1S	2.28(1)	0(1)					
1Imd	2.06(2)	8(2)					
1Imd	1.94(2)	5(2)					
1Imd	2.19(2)	6(2)	0(2)	0.0533	2293.913	212.442	9

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(4)	6(4)					
1S	2.30(1)	0(1)					
1Imd	2.06(4)	3(4)	0(2)	0.0695	2991.738	233.769	7
1N/O	2.00(2)	3(2)					
1S	2.28(1)	2(1)					
1Imd	1.89(2)	1(2)					
1Imd	2.05(2)	1(1)	neg5(2)	0.0422	1818.189	168.384	9
0N/O							
1S	2.28(1)	0(1)					
1Imd	1.94(2)	5(2)					
1Imd	2.19(2)	6(2)					
1Imd	2.06(2)	8(2)	0(2)	0.0516	2222.270	205.807	9

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(4)	2(4)					
1S	2.72(5)	6(6)					
1Imd	2.19(3)	2(3)	8(3)	0.3192	13743.811	1073.915	7
1N/O	2.13(3)	5(2)					
1S	2.66(2)	0(2)					
1Imd	1.99(2)	4(2)					
1Imd	2.12(4)	3(4)	1(3)	0.1957	8426.085	780.348	9
0N/O							
1S	2.67(3)	3(4)					
1Imd	1.95(2)	8(2)					
1Imd	2.06(2)	12(2)					
1Imd	2.18(2)	11(2)	1(2)	0.2205	9495.654	879.402	9

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(4)	2(4)					
1S	2.73(6)	7(7)					
1Imd	2.19(3)	2(3)	8(3)	0.3230	13907.802	1086.729	7
1N/O	2.13(3)	5(2)					
1S	2.66(2)	0(2)					
1Imd	1.99(2)	4(2)					
1Imd	2.12(4)	3(4)	1(3)	0.2018	8691.387	804.918	9
0N/O							
1S	2.67(3)	3(4)					
1Imd	2.06(2)	12(2)					
1Imd	2.18(2)	11(2)					
1Imd	1.95(2)	9(2)	1(2)	0.2239	9642.446	892.997	9

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.19(0.29)	31(125)					
2S	2.28(1)	3(1)					
1Imd	2.00(3)	1(2)	neg2(4)	0.0857	3691.897	288.478	7
0N/O							
2S	2.28(1)	4(1)					
1Imd	2.09(0.11)	8(23)					
1Imd	1.99(5)	2(3)	neg2(3)	0.0778	3350.056	261.767	9

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(4)	2(4)					
2S	2.28(1)	3(1)					
1Imd	2.01(7)	6(8)	neg4(2)	0.0879	3783.882	295.665	7
0N/O							
2S	2.28(1)	4(1)					
1Imd	2.08(0.13)	9(26)					
1Imd	1.99(7)	2(3)	neg3(3)	0.0788	3392.953	265.119	9

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.17(0.24)	27(102)					
2S	2.28(1)	3(1)					
1Imd	2.00(2)	2(2)	neg3(4)	0.0876	3771.209	294.675	7
0N/O							
2S	2.28(1)	4(1)					
1Imd	2.07(0.15)	10(27)					
1Imd	1.99(7)	3(3)	neg3(3)	0.0807	3474.747	271.510	9

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.18(2)	5(2)					
2S	2.91(0.19)	29(38)					
1Imd	2.07(2)	2(3)	10(0)	0.3843	16548.816	1293.093	7
0N/O							
2S	2.99(0.39)	41(84)					
1Imd	2.18(3)	6(2)					
1Imd	2.05(3)	4(2)	7(4)	0.4169	17951.015	1402.658	9

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(3)	5(2)					
2S	2.69(4)	6(4)	3(4)	0.3892	16760.003	1309.595	7

1Imd	2.04(3)	3(2)					
0N/O							
2S	2.70(4)	7(4)					
1Imd	2.16(2)	6(2)					
1Imd	2.03(3)	5(2)	3(3)	0.3951	17012.952	1329.360	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(0.27)	24(104)					
1S	2.18(2)	1(3)					
1S	2.31(2)	3(2)					
1Imd	1.97(5)	5(5)	neg6(5)	0.0563	2424.470	224.533	9
0N/O							
1S	2.17(2)	1(2)					
1S	2.30(1)	3(1)					
1Imd	1.91(3)	0(2)					
1Imd	2.06(3)	1(2)	neg6(2)	0.0380	1636.533	151.561	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	10(1)					
1S	2.11(2)	6(2)					
1S	2.30(1)	6(1)					
1Imd	1.95(3)	3(2)	neg7(3)	0.0370	1591.462	147.387	9
0N/O							
1S	2.17(2)	1(2)					
1S	2.30(1)	3(1)					
1Imd	2.06(3)	1(2)					
1Imd	1.90(3)	1(2)	neg7(2)	0.0411	1767.728	163.711	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(2)	1(2)					
1S	2.29(1)	0(0)					
1S	2.67(2)	5(2)					
1Imd	2.06(2)	2(2)	neg1(2)	0.0236	1014.319	93.937	9
0N/O							
1S	2.28(1)	0(1)					
1S	2.65(2)	4(2)					
1Imd	1.98(3)	0(4)					
1Imd	2.09(4)	0(5)	neg2(2)	0.0436	1876.321	173.768	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(2)	1(2)					
1S	2.29(1)	0(0)	neg1(2)	0.0237	1019.564	94.423	9

1S	2.67(2)	5(2)					
1Imd	2.06(2)	1(2)					
0N/O							
1S	2.28(1)	0(1)					
1S	2.66(2)	4(2)					
1Imd	2.09(5)	0(6)					
1Imd	1.98(3)	0(5)	neg2(2)	0.0447	1925.206	178.295	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.14(0.22)	20(86)					
1S	2.18(2)	1(3)					
1S	2.31(2)	2(2)					
1Imd	1.96(5)	5(5)	neg6(5)	0.0582	2506.140	232.096	9
0N/O							
1S	2.30(1)	3(1)					
1S	2.17(2)	1(2)					
1Imd	2.06(3)	1(2)					
1Imd	1.91(3)	0(2)	neg7(2)	0.0380	1636.136	151.524	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(2)	1(2)					
1S	2.29(1)	0(0)					
1S	2.66(2)	5(2)					
1Imd	2.06(3)	2(2)	neg1(2)	0.0242	1040.380	96.351	9
0N/O							
1S	2.29(1)	0(1)					
1S	2.65(2)	4(2)					
1Imd	2.09(4)	0(5)					
1Imd	1.98(3)	0(4)	neg2(2)	0.0422	1816.403	168.219	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(2)	1(2)					
1S	2.29(1)	0(0)					
1S	2.67(2)	6(2)					
1Imd	2.06(2)	2(2)	neg1(2)	0.0241	1039.284	96.249	9
0N/O							
1S	2.29(1)	0(1)					
1S	2.65(2)	4(2)					
1Imd	1.98(3)	0(4)					
1Imd	2.09(4)	0(5)	neg2(2)	0.0431	1855.774	171.865	9

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(3)	2(2)					
1S	2.66(2)	6(2)					
1S	2.29(1)	0(0)					
1Imd	2.06(3)	2(2)	neg2(2)	0.0267	1149.044	106.414	9
0N/O							
1S	2.29(1)	0(1)					
1S	2.65(2)	4(2)					
1Imd	2.09(4)	0(4)					
1Imd	1.98(3)	0(4)	neg2(2)	0.0416	1789.334	165.712	9

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(2)	1(2)					
1S	2.29(1)	0(0)					
1S	2.66(2)	6(2)					
1Imd	2.06(3)	2(2)	neg1(2)	0.0249	1071.641	99.246	9
0N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(3)	2(2)					
1S	2.66(2)	6(2)					
1S	2.29(1)	0(0)					
1Imd	2.06(3)	2(2)	neg2(2)	0.0262	1127.245	104.395	9
0N/O							
1S	2.65(2)	4(2)					
1S	2.29(1)	1(1)					
1Imd	2.09(4)	0(4)					
1Imd	1.98(3)	0(4)	neg2(2)	0.0407	1754.515	162.487	9

Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(2)	3(2)	neg3(2)	0.0225	969.051	89.745	9

1Br	2.41(1)	6(1)					
1Imd	1.97(2)	1(3)					
1Imd	2.08(3)	0(3)					

Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(2)	3(2)					
1Br	2.41(1)	6(1)					
1Imd	1.97(2)	1(3)					
1Imd	2.09(3)	0(3)	neg3(2)	0.0225	968.769	89.719	9

Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(2)	3(2)					
1Br	2.42(1)	7(1)					
1Imd	1.97(2)	1(3)					
1Imd	2.09(3)	0(3)	neg3(2)	0.0225	971.003	89.926	9

Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.08(3)	0(3)					
1Imd	1.96(2)	1(3)	neg3(2)	0.0228	981.616	90.908	9

Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	3(2)					
1Br	2.41(1)	6(1)					
1Imd	1.97(2)	0(3)					
1Imd	2.08(3)	0(3)	neg3(2)	0.0227	977.228	90.502	9

Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1S	2.28(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	1.96(2)	1(3)					
1Imd	2.08(3)	0(3)	neg3(2)	0.0236	1014.321	93.937	9

Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	2.08(3)	0(3)					
1Imd	1.96(2)	0(3)	neg3(2)	0.0232	999.114	92.529	9

Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	1.96(2)	0(3)					
1Imd	2.08(3)	0(3)	neg3(2)	0.0230	992.082	91.878	9

Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.29(1)	0(1)					
1Br	2.77(2)	7(1)					
1Imd	1.97(4)	0(5)					
1Imd	2.06(4)	1(4)	neg3(2)	0.0342	1471.488	136.276	9

Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	1.96(2)	1(3)					
1Imd	2.08(3)	0(3)	neg4(2)	0.0242	1042.335	96.532	9

Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.08(3)	0(3)					
1Imd	1.96(2)	0(3)	neg3(2)	0.0238	1024.578	94.887	9

Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	3(2)					
1Br	2.41(1)	6(1)					
1Imd	1.96(2)	0(3)					
1Imd	2.08(3)	0(3)	neg3(2)	0.0236	1015.678	94.063	9

Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.97(0.12)	15(19)					
1Br	2.42(2)	4(1)					
1Imd	1.98(2)	4(2)					
1Imd	2.11(2)	5(2)	neg1(3)	0.1089	4688.125	434.172	9

Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	4(2)					
1Br	2.40(1)	6(2)					
1Imd	1.96(2)	0(3)					
1Imd	2.08(3)	0(3)	neg4(2)	0.0239	1028.441	95.245	9

Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	4(2)					
1Br	2.40(1)	6(2)					
1Imd	2.08(3)	0(3)					
1Imd	1.96(2)	0(3)	neg4(2)	0.0236	1017.711	94.251	9

Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	1.98(0.11)	15(17)					
1Br	2.42(2)	4(1)					
1Imd	2.11(2)	5(2)					
1Imd	1.98(2)	4(2)	neg1(3)	0.1087	4680.724	433.487	9

Zn-N(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(3)	4(3)					
1Br	2.42(1)	4(1)					
1Imd	2.05(1)	4(1)	1(3)	0.0716	3085.118	241.065	7
1N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
1Br	2.41(1)	4(1)					
1Imd	2.17(3)	7(4)					
1Imd	2.05(3)	8(4)	neg1(2)	0.0805	3468.558	321.227	11

1Imd	1.94(3)	5(3)					

Zn-N(2.0) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(3)	1(3)					
1Br	2.42(1)	4(1)					
1Imd	1.97(2)	2(1)					
1Imd	2.11(2)	2(2)	neg1(2)	0.0558	2403.879	222.626	9

Zn-N(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(3)	4(3)					
1Br	2.42(1)	4(1)					
1Imd	2.05(6)	5(6)	1(3)	0.0762	3279.831	256.280	7
1N/O	2.08(2)	1(2)					
1Br	2.42(1)	4(1)					
1Imd	2.11(2)	2(2)					
1Imd	1.96(2)	2(1)	neg1(2)	0.0461	1986.076	183.933	9
0N/O							
1Br	2.41(1)	4(1)					
1Imd	2.17(3)	7(4)					
1Imd	2.05(3)	8(4)					
1Imd	1.94(3)	5(3)	neg1(2)	0.0835	3596.681	333.092	11

Zn-N(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(3)	4(3)					
1Br	2.42(1)	4(1)					
1Imd	2.05(6)	5(6)	1(3)	0.0837	3604.945	281.684	7
1N/O	2.09(2)	1(2)					
1Br	2.42(1)	4(1)					
1Imd	2.11(2)	2(2)					
1Imd	1.97(2)	2(1)	neg1(2)	0.0514	2215.402	205.171	9
0N/O							
1Br	2.42(1)	5(1)					
1Imd	2.05(3)	8(4)					
1Imd	2.17(3)	7(4)					
1Imd	1.94(3)	5(3)	neg1(2)	0.0883	3803.605	352.256	11

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(6)	14(6)					
1S	2.29(1)	0(1)					
1Imd	2.04(2)	2(3)	0(3)	0.0851	3664.769	286.358	7

2N/O	2.02(5)	10(6)					
1S	2.27(2)	1(1)					
1Imd	2.01(4)	4(4)					
1Imd	2.50(2)	1(2)	neg4(3)	0.0474	2043.082	189.212	9
1N/O	1.99(2)	2(2)					
1S	2.27(1)	1(1)					
1Imd	2.03(2)	1(2)					
1Imd	1.87(3)	1(2)					
1Imd	2.49(3)	1(3)	neg7(2)	0.0285	1227.927	139.571	11

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(6)	14(6)					
1S	2.29(1)	0(1)					
1Imd	2.04(2)	2(3)	0(3)	0.0816	3512.219	274.438	7
2N/O	2.03(4)	5(3)					
1S	2.30(1)	0(1)					
1Imd	2.35(0.20)	18(31)					
1Imd	2.08(5)	3(5)	1(3)	0.0651	2804.774	259.753	9
1N/O	1.99(2)	2(2)					
1S	2.27(1)	1(1)					
1Imd	2.48(3)	1(3)					
1Imd	1.87(3)	1(2)					
1Imd	2.03(2)	1(2)	neg7(2)	0.0281	1210.605	137.602	11

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(6)	15(6)					
1S	2.29(1)	0(1)					
1Imd	2.04(2)	2(3)	0(3)	0.0794	3419.200	267.170	7
2N/O	2.03(4)	5(4)					
1S	2.30(1)	0(1)					
1Imd	2.07(5)	3(5)					
1Imd	2.32(0.22)	21(43)	1(3)	0.0647	2785.434	257.962	9
1N/O	1.99(2)	2(2)					
1S	2.27(1)	1(1)					
1Imd	1.87(3)	1(2)					
1Imd	2.48(3)	1(3)					
1Imd	2.03(2)	1(2)	neg7(2)	0.0287	1235.462	140.428	11

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(3)	4(3)					
1S	2.70(4)	5(4)	6(3)	0.2657	11440.397	893.931	7

1Imd	2.18(3)	2(2)					
2N/O	2.12(3)	0(3)					
1S	2.66(2)	1(2)					
1Imd	1.99(3)	3(2)					
1Imd	2.14(4)	3(3)	2(3)	0.1948	8388.645	776.881	9
1N/O	2.12(3)	3(3)					
1S	2.66(2)	2(3)					
1Imd	2.05(3)	10(3)					
1Imd	2.18(3)	9(3)					
1Imd	1.94(3)	7(3)	1(2)	0.1527	6574.661	747.303	11

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(3)	4(3)					
1S	2.71(4)	6(5)					
1Imd	2.18(3)	2(2)	6(3)	0.2699	11622.407	908.153	7
2N/O	2.12(3)	1(3)					
1S	2.66(2)	1(2)					
1Imd	1.99(3)	3(2)					
1Imd	2.14(4)	3(3)	2(3)	0.2016	8679.321	803.801	9
1N/O	2.12(3)	3(3)					
1S	2.66(3)	2(3)					
1Imd	2.05(3)	10(3)					
1Imd	1.94(3)	7(3)					
1Imd	2.18(3)	9(3)	1(2)	0.1582	6813.370	774.436	11

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.21(0.16)	34(67)					
2S	2.28(2)	3(1)					
1Imd	2.00(3)	1(2)	neg2(4)	0.0826	3555.496	277.820	7
1N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
2S	2.28(2)	4(1)					
1Imd	2.22(0.41)	23(173)					
1Imd	1.99(6)	2(4)					
1Imd	2.11(0.23)	7(28)	neg1(5)	0.0736	3169.743	293.553	11

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2N/O	2.20(0.14)	31(62)					
2S	2.28(2)	3(1)					
1Imd	2.00(3)	2(2)	neg2(4)	0.0827	3563.194	278.421	7
1N/O	2.10(0.17)	19(44)					
2S	2.25(2)	5(1)					
1Imd	1.96(3)	4(3)					
1Imd	2.48(2)	1(2)	neg7(3)	0.0559	2408.448	223.049	9
0N/O							
2S	2.28(2)	4(1)					
1Imd	2.19(0.57)	21(162)					
1Imd	1.99(7)	2(5)					
1Imd	2.11(0.32)	8(31)	neg1(4)	0.0746	3212.544	297.517	11

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.19(0.14)	30(58)					
2S	2.28(2)	3(1)					
1Imd	2.00(3)	2(2)	neg2(4)	0.0838	3609.311	282.025	7
1N/O	2.46(1)	3(1)					
2S	2.26(2)	7(2)					
1Imd	1.93(3)	1(3)					
1Imd	2.06(3)	0(3)	neg7(2)	0.0402	1730.874	160.298	9
0N/O							
2S	2.28(2)	4(1)					
1Imd	1.99(7)	2(6)					
1Imd	2.16(0.85)	18(156)					
1Imd	2.11(0.58)	9(51)	neg1(4)	0.0765	3294.726	305.128	11

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(3)	2(4)					
2S	2.76(6)	12(7)					
1Imd	2.19(3)	2(2)	8(3)	0.3248	13987.902	1092.988	7
1N/O	2.15(4)	2(4)					
2S	2.91(0.24)	33(49)					
1Imd	2.18(5)	3(3)					
1Imd	2.03(3)	3(2)	7(4)	0.2991	12879.192	1192.755	9
0N/O							
2S	3.07(5)	8(6)					
1Imd	2.07(2)	13(2)					
1Imd	1.95(3)	9(2)					
1Imd	2.19(2)	12(2)	2(3)	0.2415	10400.424	963.194	11

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(3)	2(4)					
2S	2.76(6)	12(7)					
1Imd	2.19(3)	2(2)	8(3)	0.3308	14244.583	1113.045	7
1N/O	2.14(4)	3(4)					
2S	2.69(4)	7(4)					
1Imd	2.15(4)	3(4)					
1Imd	2.01(3)	4(2)	3(3)	0.2920	12575.188	1164.601	9
0N/O							
2S	2.70(5)	11(6)					
1Imd	2.06(2)	12(2)					
1Imd	1.95(3)	8(3)					
1Imd	2.19(2)	11(2)	1(3)	0.2689	11577.967	1072.247	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.17(0.13)	26(59)					
1S	2.19(2)	1(3)					
1S	2.31(2)	2(2)					
1Imd	1.98(6)	5(5)	neg4(6)	0.0538	2317.587	214.634	9
1N/O	2.26(4)	7(2)					
1S	2.19(4)	1(5)					
1S	2.28(4)	4(3)					
1Imd	1.93(3)	1(2)					
1Imd	2.08(3)	1(2)	neg5(2)	0.0224	965.210	109.710	11
0N/O							
1S	2.18(2)	0(2)					
1S	2.31(1)	3(1)					
1Imd	2.06(3)	4(3)					
1Imd	2.20(5)	0(6)					
1Imd	1.93(3)	1(2)	neg3(2)	0.0364	1566.336	178.036	11

Zn-N(2.2) Zn-S(2.2) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.23(6)	6(9)					
1S	2.18(8)	2(6)					
1S	2.29(7)	3(10)					
1Imd	1.94(2)	5(2)					
1Imd	2.09(2)	6(1)	neg4(2)	0.0243	1047.654	119.081	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.17(0.14)	25(58)					
1S	2.19(2)	1(3)					
1S	2.31(2)	2(2)	neg5(6)	0.0550	2367.048	219.215	9

1Imd	1.98(6)	5(5)					
1N/O	2.27(5)	7(3)					
1S	2.29(5)	5(4)					
1S	2.19(3)	2(5)					
1Imd	1.93(3)	1(1)					
1Imd	2.08(3)	2(2)	neg5(2)	0.0222	956.356	108.703	11
0N/O							
1S	2.18(2)	0(3)					
1S	2.31(1)	2(2)					
1Imd	1.93(3)	1(3)					
1Imd	2.06(3)	4(3)					
1Imd	2.20(5)	1(6)	neg3(2)	0.0394	1696.850	192.871	11

Zn-N(2.2) Zn-S(2.2) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(2)	10(2)					
1S	2.30(1)	6(1)					
1S	2.13(2)	6(2)					
1Imd	1.91(4)	3(6)					
1Imd	2.05(4)	1(5)	neg5(2)	0.0209	901.589	102.478	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(2)	6(2)					
1S	2.29(1)	0(0)					
1S	2.66(1)	5(1)					
1Imd	2.06(2)	2(2)	neg1(1)	0.0179	771.529	71.452	9
1N/O	2.01(2)	1(3)					
1S	2.29(1)	0(1)					
1S	2.66(2)	5(2)					
1Imd	2.02(0.15)	10(15)					
1Imd	2.08(6)	3(4)	neg1(2)	0.0147	633.790	72.039	11
0N/O							
1S	2.28(1)	1(1)					
1S	2.65(2)	5(2)					
1Imd	1.94(2)	4(2)					
1Imd	2.06(2)	7(2)					
1Imd	2.19(2)	5(3)	0(2)	0.0273	1174.814	133.534	11

Zn-N(2.2) Zn-S(2.2) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(2)	2(3)					
1S	2.29(1)	1(1)					
1S	2.66(2)	5(2)					
1Imd	2.06(0.18)	11(14)	neg1(2)	0.0143	613.917	69.780	11

1Imd	2.06(7)	4(6)					

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(2)	6(2)					
1S	2.29(1)	0(0)					
1S	2.66(1)	5(2)					
1Imd	2.06(2)	2(2)	neg1(1)	0.0184	791.875	73.336	9
1N/O	2.01(2)	1(3)					
1S	2.29(1)	0(1)					
1S	2.66(2)	6(2)					
1Imd	2.08(6)	3(4)					
1Imd	2.01(0.15)	10(14)	neg1(2)	0.0154	662.189	75.267	11
0N/O							
1S	2.28(1)	0(1)					
1S	2.66(2)	6(2)					
1Imd	1.94(2)	4(2)					
1Imd	2.19(2)	5(3)					
1Imd	2.06(2)	7(2)	0(2)	0.0286	1233.492	140.204	11

Zn-N(2.2) Zn-S(2.2) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(1)	1(1)					
1S	2.29(2)	2(3)					
1S	2.66(2)	5(2)					
1Imd	2.06(0.18)	11(14)					
1Imd	2.06(6)	4(5)	neg1(2)	0.0149	642.373	73.015	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(0.12)	24(53)					
1S	2.19(2)	1(3)					
1S	2.31(2)	2(2)					
1Imd	1.98(6)	5(5)	neg5(6)	0.0555	2387.829	221.139	9
1N/O	2.08(3)	9(2)					
1S	2.30(1)	5(1)					
1S	2.11(3)	4(2)					
1Imd	1.97(3)	2(4)					
1Imd	2.13(4)	0(5)	neg3(2)	0.0265	1141.353	129.731	11
0N/O							
1S	2.31(1)	3(2)					
1S	2.18(2)	0(3)					
1Imd	1.93(3)	1(3)					
1Imd	2.06(3)	3(3)					
1Imd	2.19(5)	1(8)	neg4(2)	0.0373	1606.372	182.587	11

Zn-N(2.2) Zn-S(2.3) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(2)	6(2)					
1S	2.29(1)	0(0)					
1S	2.66(1)	5(2)					
1Imd	2.06(2)	2(2)	neg1(1)	0.0174	748.420	69.312	9
1N/O	2.01(2)	2(3)					
1S	2.29(1)	0(1)					
1S	2.66(1)	6(2)					
1Imd	2.01(0.11)	8(13)					
1Imd	2.09(7)	3(5)	neg1(2)	0.0138	594.098	67.528	11
0N/O							
1S	2.28(1)	1(1)					
1S	2.65(2)	6(2)					
1Imd	2.19(2)	5(2)					
1Imd	1.94(2)	4(2)					
1Imd	2.06(2)	7(2)	0(1)	0.0253	1087.582	123.619	11

Zn-N(2.2) Zn-S(2.3) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	2(3)					
1S	2.66(1)	5(2)					
1S	2.29(1)	1(1)					
1Imd	2.04(0.26)	8(26)					
1Imd	2.07(0.22)	5(9)	neg1(2)	0.0134	577.639	65.657	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(2)	6(2)					
1S	2.29(1)	0(0)					
1S	2.66(1)	6(2)					
1Imd	2.06(2)	2(2)	neg1(1)	0.0178	763.019	70.664	9
1N/O	2.01(2)	1(3)					
1S	2.29(1)	0(1)					
1S	2.66(2)	6(2)					
1Imd	2.01(0.12)	9(13)					
1Imd	2.09(6)	3(5)	neg1(2)	0.0143	617.408	70.177	11

0N/O							
1S	2.28(1)	1(1)					
1S	2.65(2)	6(2)					
1Imd	2.06(2)	7(2)					
1Imd	2.19(2)	5(2)					
1Imd	1.94(2)	4(2)	0(1)	0.0264	1136.554	129.185	11

Zn-N(2.2) Zn-S(2.3) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(2)	2(3)					
1S	2.29(1)	1(1)					
1S	2.66(1)	6(2)					
1Imd	2.04(0.19)	9(18)					
1Imd	2.07(0.11)	5(7)	neg1(2)	0.0140	601.649	68.386	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(4)	5(3)					
1S	1.95(0.19)	32(39)					
1S	2.30(1)	0(1)					
1Imd	2.08(5)	3(4)	1(5)	0.0613	2637.741	244.284	9
1N/O	2.01(2)	2(3)					
1S	2.29(1)	0(1)					
1S	2.65(1)	6(2)					
1Imd	2.09(7)	3(5)					
1Imd	2.00(0.10)	7(11)	neg1(2)	0.0135	580.318	65.961	11
0N/O							
1S	2.28(1)	1(1)					
1S	2.65(2)	6(2)					
1Imd	1.94(2)	4(2)					
1Imd	2.19(2)	5(2)					
1Imd	2.06(2)	7(2)	0(1)	0.0241	1036.726	117.838	11

Zn-N(2.2) Zn-S(2.4) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	3(3)					
1S	2.29(1)	1(1)					
1S	2.65(1)	6(2)					
1Imd	2.09(0.22)	5(12)					
1Imd	2.02(0.20)	6(24)	neg1(2)	0.0131	565.720	64.302	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(2)	6(2)					
1S	2.29(1)	0(0)					
1S	2.66(1)	6(2)	neg1(1)	0.0176	757.675	70.169	9

1Imd	2.06(2)	2(2)					
1N/O	2.01(2)	2(3)					
1S	2.29(1)	0(1)					
1S	2.66(2)	6(2)					
1Imd	2.09(7)	3(5)					
1Imd	2.00(0.10)	7(12)	neg1(2)	0.0139	600.139	68.214	11
0N/O							
1S	2.28(1)	1(1)					
1S	2.65(2)	6(2)					
1Imd	1.94(2)	4(2)					
1Imd	2.06(2)	7(2)					
1Imd	2.19(2)	5(2)	0(1)	0.0251	1078.984	122.642	11

Zn-N(2.2) Zn-S(2.4) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	2(3)					
1S	2.29(1)	1(1)					
1S	2.66(1)	6(2)					
1Imd	2.08(0.27)	5(11)					
1Imd	2.03(0.27)	7(29)	neg1(2)	0.0136	586.465	66.660	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(2)	7(2)					
1S	2.65(1)	6(2)					
1S	2.29(1)	0(0)					
1Imd	2.05(2)	3(2)	neg2(2)	0.0172	742.601	68.773	9
1N/O	2.02(2)	2(3)					
1S	2.65(1)	6(2)					
1S	2.29(1)	0(1)					
1Imd	1.99(7)	6(9)					
1Imd	2.09(5)	3(5)	neg2(2)	0.0131	566.097	64.345	11
0N/O							
1S	2.65(2)	6(2)					
1S	2.28(1)	1(1)					
1Imd	2.06(2)	7(2)					
1Imd	1.95(2)	4(2)					
1Imd	2.19(2)	5(2)	0(1)	0.0227	975.793	110.913	11

Zn-N(2.2) Zn-S(2.5) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	3(3)					
1S	2.65(1)	6(2)					
1S	2.29(1)	1(1)					
1Imd	2.01(9)	5(13)	neg2(2)	0.0128	549.435	62.451	11

1Imd	2.09(0.10)	4(8)					

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(4)	6(5)					
1S	2.28(2)	4(2)					
1Br	2.41(1)	7(1)					
1Imd	1.99(3)	3(5)					
1Imd	2.11(4)	3(5)	neg2(1)	0.0110	475.202	54.013	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	6(5)					
1S	2.28(1)	3(2)					
1Br	2.41(1)	7(1)					
1Imd	2.11(4)	3(6)					
1Imd	1.99(3)	3(5)	neg2(1)	0.0109	469.229	53.335	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	1(2)					
1S	2.28(1)	1(1)					
1Br	2.81(2)	7(1)					
1Imd	2.19(4)	1(4)					
1Imd	2.05(2)	3(2)	0(2)	0.0167	719.959	81.834	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(4)	6(5)					
1S	2.29(2)	4(2)					
1Br	2.41(1)	6(1)					
1Imd	1.98(3)	3(4)	neg2(1)	0.0110	473.725	53.846	11

1Imd	2.11(3)	3(4)					

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(4)	6(5)					
1S	2.29(1)	4(2)					
1Br	2.41(1)	7(1)					
1Imd	2.11(4)	3(5)					
1Imd	1.99(3)	3(4)	neg2(1)	0.0108	466.310	53.003	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	6(5)					
1S	2.29(1)	3(2)					
1Br	2.41(1)	7(1)					
1Imd	1.99(3)	3(5)					
1Imd	2.11(4)	3(5)	neg2(1)	0.0107	461.706	52.479	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	6(5)					
1S	2.29(2)	5(2)					
1Br	2.40(1)	6(1)					
1Imd	1.98(3)	3(4)					
1Imd	2.10(3)	2(4)	neg2(2)	0.0115	494.360	56.191	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(4)	6(5)					
1S	2.29(1)	4(2)					
1Br	2.41(1)	7(1)					
1Imd	1.98(3)	3(4)					
1Imd	2.11(3)	3(4)	neg2(1)	0.0110	473.129	53.778	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	1(3)					
1S	2.29(1)	1(1)					
1Br	2.81(2)	7(2)					
1Imd	2.04(2)	2(2)	0(2)	0.0188	809.270	91.985	11

1Imd	2.17(4)	3(6)					

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	6(5)					
1S	2.29(2)	5(3)					
1Br	2.40(1)	6(1)					
1Imd	1.97(3)	3(3)					
1Imd	2.10(3)	2(3)	neg2(2)	0.0117	504.997	57.400	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	6(5)					
1S	2.29(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.10(3)	2(3)					
1Imd	1.98(3)	3(4)	neg2(2)	0.0114	491.124	55.823	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	6(5)					
1S	2.29(2)	4(2)					
1Br	2.41(1)	7(1)					
1Imd	1.98(3)	3(4)					
1Imd	2.10(3)	2(4)	neg2(1)	0.0112	482.497	54.843	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	6(5)					
1S	2.29(1)	4(2)					
1Br	2.41(1)	7(1)					
1Imd	2.11(3)	2(4)					
1Imd	1.98(3)	3(4)	neg2(1)	0.0111	477.036	54.222	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	2(2)					
1S	2.90(6)	13(10)					
1Br	2.42(1)	3(1)					
1Imd	2.10(3)	2(2)					
1Imd	1.95(2)	2(1)	neg1(2)	0.0393	1690.273	192.124	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	6(5)					
1S	2.29(2)	5(2)					
1Br	2.40(1)	6(1)					
1Imd	1.97(3)	3(3)	neg2(2)	0.0116	498.177	56.625	11

1Imd	2.10(3)	2(3)					

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	2(2)					
1S	2.88(5)	10(8)					
1Br	2.42(1)	3(1)					
1Imd	2.10(3)	2(2)					
1Imd	1.95(2)	2(1)	neg1(2)	0.0421	1813.447	206.124	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	6(5)					
1S	2.29(2)	4(2)					
1Br	2.41(1)	7(1)					
1Imd	2.10(3)	2(4)					
1Imd	1.98(3)	3(4)	neg2(2)	0.0112	482.976	54.897	11

Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.28(1)	10(2)					
1Br	2.39(1)	5(1)					
1Imd	1.96(2)	2(2)					
1Imd	2.08(2)	1(2)	neg4(1)	0.0137	589.099	54.557	9

Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.28(1)	9(2)					
1Br	2.40(1)	5(1)					
1Imd	1.96(2)	2(2)					
1Imd	2.09(2)	1(2)	neg4(1)	0.0130	558.793	51.750	9

Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.28(1)	9(2)					
1Br	2.40(1)	6(1)					
1Imd	2.09(2)	1(2)					
1Imd	1.96(2)	1(2)	neg4(1)	0.0125	540.373	50.044	9

Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.28(1)	9(2)					
1Br	2.40(1)	6(1)					
1Imd	2.09(2)	1(2)					
1Imd	1.96(2)	1(2)	neg3(1)	0.0123	528.146	48.912	9
1S	2.26(1)	4(1)					
1Br	2.74(2)	9(2)	neg8(2)	0.0256	1103.972	125.482	11

1Imd	2.00(3)	1(2)					
1Imd	1.92(7)	8(11)					
1Imd	2.47(3)	2(3)					

Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(1)	10(2)					
1Br	2.39(1)	5(1)					
1Imd	1.96(2)	1(2)					
1Imd	2.08(2)	1(2)	neg4(1)	0.0137	590.707	54.706	9

Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(1)	10(2)					
1Br	2.40(1)	6(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.96(2)	1(2)	neg4(1)	0.0132	567.746	52.580	9

Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.27(1)	4(1)					
1Br	2.75(2)	8(2)					
1Imd	2.00(0.12)	9(11)					
1Imd	2.00(4)	2(3)	neg5(2)	0.0391	1684.628	156.015	9

Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(1)	10(2)					
1Br	2.39(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.96(2)	1(2)	neg4(1)	0.0147	630.960	58.434	9

Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2S	2.29(1)	10(2)					
1Br	2.39(1)	5(1)					
1Imd	1.96(2)	1(2)					
1Imd	2.08(2)	1(2)	neg4(1)	0.0140	604.983	56.028	9

Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.27(1)	4(1)					
1Br	2.75(2)	8(2)					
1Imd	2.00(3)	2(3)					
1Imd	1.99(0.12)	9(11)	neg5(2)	0.0405	1744.230	161.535	9

Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(2)	11(2)					
1Br	2.39(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.95(2)	1(2)	neg4(2)	0.0167	718.357	66.528	9

Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(2)	10(2)					
1Br	2.39(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.95(2)	1(2)	neg4(2)	0.0157	674.854	62.499	9

Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(1)	10(2)					
1Br	2.39(1)	5(1)					
1Imd	2.08(2)	1(2)					
1Imd	1.96(2)	1(2)	neg4(1)	0.0150	646.381	59.862	9

Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.96(9)	21(15)					
1Br	2.42(2)	4(1)					
1Imd	2.11(2)	5(2)					
1Imd	1.98(2)	4(2)	neg2(3)	0.1057	4551.009	421.474	9

Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.98(9)	21(15)					
1Br	2.41(2)	3(1)					
1Imd	2.11(2)	5(2)					
1Imd	1.98(2)	3(2)	neg2(3)	0.0991	4265.409	395.024	9

Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(2)	11(2)					
1Br	2.39(1)	5(1)					
1Imd	1.95(2)	1(2)					
1Imd	2.08(2)	1(2)	neg5(2)	0.0164	704.559	65.250	9

Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.97(9)	21(15)					
1Br	2.42(2)	4(1)					
1Imd	1.98(2)	4(2)					
1Imd	2.11(2)	5(2)	neg1(3)	0.1040	4476.886	414.609	9

Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.77(8)	10(12)					
1Br	2.77(6)	6(5)					
1Imd	2.02(3)	5(2)					
1Imd	2.16(3)	6(2)	3(4)	0.3448	14846.630	1374.961	9

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	3(3)					
1S	2.38(4)	5(9)					
1Br	2.40(2)	4(2)					
1Imd	2.09(2)	1(2)					
1Imd	1.96(2)	1(2)	neg4(2)	0.0126	542.792	61.696	11

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	11

1Imd							
1Imd							

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	3(3)					
1S	2.39(4)	6(10)					
1Br	2.40(2)	4(2)					
1Imd	1.96(2)	1(2)					
1Imd	2.09(2)	1(2)	neg4(2)	0.0127	545.460	61.999	11

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(3)	3(4)					
1S	2.38(4)	6(9)					
1Br	2.40(2)	4(2)					
1Imd	1.96(2)	1(2)					
1Imd	2.09(2)	1(2)	neg4(1)	0.0123	531.700	60.435	11

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(3)	4(4)					
1S	2.37(4)	6(9)					
1Br	2.40(2)	4(2)					
1Imd	2.09(2)	1(2)					
1Imd	1.96(2)	1(2)	neg4(1)	0.0122	525.277	59.705	11

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.17(3)	5(5)					
1S	2.29(1)	1(1)					
1Br	2.77(2)	9(2)					
1Imd	1.96(5)	5(6)					
1Imd	2.06(3)	0(2)	neg6(2)	0.0218	940.617	106.914	11

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	11

1Imd							
1Imd							

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(1)	0(1)					
1S	2.76(6)	10(10)					
1Br	2.76(3)	6(2)					
1Imd	2.06(6)	0(6)					
1Imd	1.98(5)	0(6)	neg3(2)	0.0275	1184.110	134.591	11

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(3)	4(4)					
1S	2.38(5)	8(12)					
1Br	2.41(2)	4(2)					
1Imd	2.09(2)	1(3)					
1Imd	1.96(2)	1(2)	neg4(1)	0.0124	533.462	60.635	11

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	11

1Imd							
1Imd							

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	3(3)					
1S	2.38(4)	5(8)					
1Br	2.40(2)	4(2)					
1Imd	1.96(2)	1(2)					
1Imd	2.09(2)	1(2)	neg4(1)	0.0123	531.711	60.436	11

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.30(1)	1(1)					
1S	2.18(2)	4(5)					
1Br	2.78(2)	9(3)					
1Imd	1.95(5)	4(4)					
1Imd	2.06(3)	0(2)	neg6(2)	0.0209	900.462	102.350	11

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	2(3)					
1S	2.40(4)	5(9)					
1Br	2.40(2)	3(2)					
1Imd	1.95(2)	1(2)					
1Imd	2.09(2)	1(2)	neg4(2)	0.0129	557.403	63.357	11

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	11

1Imd							
1Imd							

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(1)	0(1)					
1S	2.75(6)	11(11)					
1Br	2.76(3)	7(2)					
1Imd	2.07(5)	0(5)					
1Imd	1.98(4)	0(6)	neg3(2)	0.0278	1196.689	136.021	11

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	2(3)					
1S	2.41(4)	6(10)					
1Br	2.41(2)	3(2)					
1Imd	2.09(2)	1(2)					
1Imd	1.95(2)	1(2)	neg4(2)	0.0129	557.571	63.376	11

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(3)	3(3)					
1S	2.39(4)	6(10)					
1Br	2.41(2)	4(2)					
1Imd	1.96(2)	1(2)					
1Imd	2.09(2)	1(2)	neg4(1)	0.0126	540.434	61.428	11

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(1)	0(1)					
1S	2.76(6)	12(11)					
1Br	2.76(3)	7(2)	neg3(2)	0.0278	1197.946	136.163	11

1Imd	1.98(4)	0(6)					
1Imd	2.07(5)	0(5)					

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.39(4)	3(6)					
1S	2.22(2)	2(3)					
1Br	2.40(2)	4(2)					
1Imd	1.96(2)	0(2)					
1Imd	2.09(2)	1(2)	neg4(2)	0.0130	558.060	63.431	11

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(1)	0(1)					
1S	2.74(6)	12(12)					
1Br	2.76(3)	7(2)					
1Imd	1.97(3)	0(5)					
1Imd	2.07(5)	0(4)	neg3(2)	0.0283	1220.431	138.719	11

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	2(3)					
1S	2.41(4)	5(9)					
1Br	2.41(2)	3(2)					
1Imd	2.09(2)	1(2)					
1Imd	1.95(2)	0(2)	neg4(2)	0.0132	569.007	64.676	11

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	11

1Imd							
1Imd							

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(1)	0(1)					
1S	2.75(6)	13(12)					
1Br	2.76(3)	7(2)					
1Imd	2.07(5)	0(4)					
1Imd	1.97(3)	0(5)	neg3(2)	0.0283	1219.473	138.610	11

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	2(3)					
1S	2.41(4)	4(8)					
1Br	2.40(2)	3(2)					
1Imd	2.09(2)	0(2)					
1Imd	1.95(2)	0(2)	neg4(2)	0.0136	586.068	66.615	11

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	2(3)					
1S	2.40(4)	4(8)					
1Br	2.40(2)	3(2)					
1Imd	2.09(2)	1(2)					
1Imd	1.95(2)	0(2)	neg4(2)	0.0133	572.931	65.122	11

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(2)	3(2)					
1S	2.99(5)	13(8)					
1Br	2.41(1)	6(1)					
1Imd	2.08(3)	1(3)					
1Imd	1.96(2)	0(3)	neg4(2)	0.0213	915.565	104.067	11

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.98(5)	13(7)					
1S	2.28(2)	3(2)					
1Br	2.41(1)	7(1)	neg4(2)	0.0209	898.071	102.078	11

1Imd	1.96(2)	0(3)					
1Imd	2.08(3)	0(3)					

Zn-N(2.2) Zn-S(2.3) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.24(1)	7(1)					
1S	1.86(0.24)	58(59)					
2S	2.24(1)	1(1)					
1Imd	2.08(3)	5(2)					
1Imd	1.94(3)	3(2)					
1Imd	2.21(4)	2(4)	neg1(2)	0.0186	800.694	117.786	13
1N/O	2.25(1)	10(2)					
2S	2.25(6)	24(11)					
1S	2.24(1)	6(2)					
1Imd	2.08(3)	7(2)					
1Imd	2.20(4)	4(4)					
1Imd	1.94(2)	6(2)	neg1(2)	0.0266	1144.953	168.429	13

APPENDIX G

ADDITIONAL FIT TABLES FOR GLUTAMATE 63 MUTATIONS

Table G.1. Additional Fits for Ni(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	2(2)	3(5)	0.2167	773.236	113.763	3
3N/O	2.06(2)	5(1)	3(3)	0.1135	404.910	59.573	3
4N/O	2.06(2)	7(1)	2(2)	0.0739	263.514	38.770	3
5N/O	2.06(2)	9(1)	2(2)	0.0714	254.788	37.486	3
6N/O	2.06(2)	11(2)	2(2)	0.0901	321.297	47.271	3
7N/O	2.06(2)	13(2)	1(2)	0.1194	426.132	62.695	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.15(4)	7(2)	neg19(8)	0.2506	894.110	131.547	3
3S	2.16(3)	10(2)	neg18(6)	0.1948	694.957	102.247	3
4S	2.16(3)	12(2)	neg18(6)	0.1747	623.393	91.718	3
5S	2.17(3)	15(2)	neg18(5)	0.1706	608.603	89.542	3
6S	2.17(4)	17(2)	neg18(5)	0.1738	620.136	91.238	3
7S	2.18(4)	19(2)	neg17(5)	0.1805	643.993	94.748	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.01(2)	1(1)					
1N/O	2.15(2)	3(2)	2(2)	0.0605	215.713	44.970	5
2N/O	2.00(2)	2(2)					
2N/O	2.13(3)	3(3)	2(2)	0.0566	201.833	42.076	5
3N/O	2.03(2)	3(2)					
1N/O	2.16(3)	0(3)	2(2)	0.0581	207.153	43.185	5
4N/O	2.06(2)	6(2)					
1N/O	2.27(0.10)	10(15)	4(3)	0.0567	202.453	42.205	5
3N/O	2.05(2)	5(2)					
2N/O	2.19(9)	16(14)	4(3)	0.0563	201.006	41.904	5
5N/O	2.08(2)	8(1)					
1N/O	2.34(6)	7(8)	4(2)	0.0566	201.806	42.070	5
4N/O	2.07(2)	7(2)		0.0539			
2N/O	2.29(7)	16(12)	5(2)		192.418	40.113	5

3N/O	2.06(2)	5(2)					
3N/O	2.23(9)	23(14)	5(3)	0.0559	199.587	41.608	5
6N/O	2.08(2)	11(2)					
1N/O	2.37(5)	4(6)	4(2)	0.0672	239.888	50.009	5
5N/O	2.08(2)	8(1)					
2N/O	2.34(5)	12(8)	5(2)	0.0601	214.406	44.697	5
4N/O	2.07(2)	7(2)					
3N/O	2.30(7)	22(13)	6(2)	0.0584	208.296	43.423	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.14(5)	6(3)					
1S	2.28(9)	5(7)	neg16(8)	0.1737	619.565	129.160	5
2S	2.29(8)	11(9)					
2S	2.15(4)	6(4)	neg14(7)	0.1480	528.126	110.098	5
3S	2.17(4)	8(2)					
1S	2.36(8)	7(7)	neg13(6)	0.1413	504.094	105.088	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.18(3)	8(2)					
2S	2.37(6)	11(6)	neg11(5)	0.1099	392.085	81.738	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.19(3)	10(2)					
2S	2.41(4)	10(4)	neg10(4)	0.0909	324.288	67.604	5
3S	2.36(5)	13(5)					
3S	2.18(3)	8(2)	neg10(5)	0.1008	359.522	74.949	5
6S	2.14(5)	14(3)					
1S	1.87(8)	13(10)	neg22(9)	0.1554	554.500	115.596	5
5S	2.21(3)	12(2)					
2S	2.43(4)	9(3)	neg10(3)	0.0800	285.461	59.510	5
4S	2.37(4)	15(5)					
3S	2.18(2)	8(2)	neg9(4)	0.0846	301.854	62.927	5

Ni-N(2.0) Ni-S(2.2)							
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.02(4)	3(2)					5
1S	2.30(8)	10(8)	neg2(6)	0.1492	532.220	110.951	
1N/O	1.97(5)	1(3)					5
2S	2.22(6)	9(4)	neg10(8)	0.1714	611.447	127.468	
2N/O							
2S							5
3N/O	2.06(2)	5(1)					
1S	2.47(0.10)	18(14)	3(3)	0.0743	265.246	55.296	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.06(1)	7(1)					
1S	2.52(6)	16(8)	3(2)	0.0449	160.340	33.426	5
2N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.05(2)	5(1)					
2S	2.47(8)	26(11)	3(3)	0.0605	215.899	45.008	5
5N/O	2.05(3)	9(3)					
1S	1.91(7)	15(12)	4(2)	0.0528	188.505	39.297	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.06(1)	7(1)					
2S	2.52(7)	25(10)	3(2)	0.0420	149.960	31.262	5
2N/O	2.63(5)	4(5)					
4S	2.18(3)	12(2)	neg14(4)	0.1021	364.261	75.937	5
3N/O	1.80(0.23)	28(48)					
3S	2.15(5)	10(3)	neg20(11)	0.1751	624.564	130.202	5
6N/O	2.03(3)	12(5)					
1S	1.90(6)	11(5)	3(2)	0.0539	192.145	40.056	5
1N/O	2.64(5)	0(5)					
6S	2.18(3)	17(2)	neg15(4)	0.1194	425.813	88.769	5

5N/O	2.06(2)	9(1)					
2S	2.56(7)	24(10)	3(2)	0.0522	186.381	38.855	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.06(2)	7(1)					
3S	2.53(7)	32(11)	3(2)	0.0421	150.095	31.290	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(6)	3(4)					5
1Br	2.03(0.14)	19(22)	1(7)	0.1944	693.549	144.584	
1N/O	2.05(6)	0(4)					5
2Br	2.50(0.32)	29(40)	4(15)	0.4237	1511.620	315.126	
2N/O	2.03(5)	3(3)					
2Br	2.04(0.11)	24(16)	1(6)	0.1895	675.995	140.924	5
3N/O	2.05(3)	5(2)					
1Br	2.15(0.28)	30(47)	2(4)	0.1080	385.254	80.313	5
1N/O	2.05(6)	0(4)					
3Br	2.53(0.32)	32(40)	4(15)	0.4221	1506.110	313.977	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.07(2)	6(2)					
1Br	2.26(0.10)	20(13)	3(2)	0.0631	225.165	46.940	5
2N/O	2.03(4)	3(3)					
3Br	2.05(0.11)	28(16)	1(6)	0.1873	668.191	139.297	5
3N/O	2.05(3)	4(2)					
2Br	2.15(0.20)	35(33)	2(3)	0.1048	373.785	77.923	5
5N/O	2.08(2)	8(2)					
1Br	2.28(5)	16(7)	3(2)	0.0520	185.345	38.639	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.06(2)	6(2)					
2Br	2.24(0.11)	29(15)	2(2)	0.0617	220.113	45.887	5

2N/O	2.03(4)	3(3)					
4Br	2.06(0.11)	32(15)	1(6)	0.1858	662.797	138.173	5
3N/O	2.05(2)	5(2)					
3Br	2.16(0.17)	38(29)	2(3)	0.1025	365.573	76.211	5
6N/O	2.08(2)	11(2)					
1Br	2.30(4)	14(5)	3(2)	0.0622	221.840	46.247	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.07(2)	8(1)					
2Br	2.27(7)	24(8)	3(2)	0.0527	188.095	39.212	5
2N/O	2.03(4)	3(3)					
5Br	2.06(0.11)	34(15)	1(6)	0.1845	658.378	137.251	5
4N/O	2.06(2)	6(2)					
3Br	2.23(0.11)	33(15)	2(2)	0.0603	215.086	44.839	5
3N/O	2.05(2)	5(2)					
4Br	2.16(0.15)	40(26)	2(3)	0.1007	359.161	74.874	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	5(1)					
1S	2.55(2)	6(2)					
1Br	2.50(2)	1(2)	5(1)	0.0143	51.166	18.294	7
3N/O	2.03(2)	5(2)					
2S	2.41(6)	10(7)					
1Br	2.36(5)	8(5)	0(3)	0.0368	131.293	46.943	7
3N/O	2.04(3)	3(2)					
1S	2.29(4)	0(3)					
2Br	2.24(5)	9(4)	neg1(3)	0.0445	158.795	56.776	7

Table G.2. Additional Fits for Ni(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Ni-N(2.0)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.07(2)	3(2)	5(4)	0.2871	3347.714	199.294	3
3N/O	2.07(2)	5(1)	5(2)	0.1901	2216.941	131.978	3
4N/O	2.07(2)	7(1)	4(2)	0.1514	1765.997	105.132	3
5N/O	2.07(2)	9(1)	4(2)	0.1472	1716.278	102.172	3

6N/O	2.07(2)	11(1)	3(2)	0.1626	1896.582	112.906	3
7N/O	2.07(2)	14(2)	3(2)	0.1885	2198.211	130.863	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(3)	7(2)	-14(6)	0.3064	3572.621	212.683	3
3S	2.18(3)	10(1)	-15(5)	0.2486	2898.347	172.543	3
4S	2.18(3)	13(1)	-15(4)	0.2262	2637.420	157.009	3
5S	2.18(3)	15(2)	-15(4)	0.2205	2571.761	153.101	3
6S	2.19(3)	17(2)	-15(4)	0.2233	2603.256	154.976	3
7S	2.19(3)	19(2)	-15(4)	0.2302	2683.869	159.775	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.02(2)	0(2)					
1N/O	2.15(2)	2(2)	4(2)	0.1567	1826.661	123.441	5
2N/O	2.01(3)	3(3)					
2N/O	2.13(3)	3(3)	3(2)	0.1447	1686.732	113.985	5
3N/O	2.04(2)	4(2)					
1N/O	2.16(3)	1(3)	3(2)	0.1431	1668.615	112.761	5
4N/O	2.08(2)	7(2)					
1N/O	2.31(0.14)	18(31)	6(2)	0.1407	1640.227	110.842	5
3N/O	2.07(2)	6(2)					
2N/O	2.17(0.17)	22(18)	5(3)	0.1457	1699.512	114.849	5
5N/O	2.09(2)	9(1)					
1N/O	2.41(6)	8(8)	6(2)	0.1323	1542.180	104.216	5
4N/O	2.08(2)	7(1)					
2N/O	2.34(8)	21(17)	7(2)	0.1345	1568.498	105.995	5
3N/O	2.07(2)	5(1)					
3N/O	2.25(0.13)	31(20)	6(3)	0.1427	1663.637	112.424	5
6N/O	2.09(2)	11(1)					
1N/O	2.42(4)	5(5)	6(2)	0.1368	1594.669	107.764	5
5N/O	2.09(2)	9(1)					
2N/O	2.41(5)	13(8)	7(2)	0.1293	1507.339	101.862	5
4N/O	2.09(2)	7(1)					
3N/O	2.36(6)	26(14)	8(2)	0.1323	1542.137	104.214	5

Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2S	2.14(4)	6(3)					
1S	2.27(6)	5(5)	-14(6)	0.2387	2783.201	188.081	5
2S	2.16(4)	8(4)					
2S	2.28(8)	13(10)	-12(5)	0.2157	2515.321	169.979	5
3S	2.18(3)	9(3)					
1S	2.34(9)	10(10)	-12(5)	0.2162	2521.266	170.381	5
4S	2.20(3)	11(2)					
1S	2.41(6)	9(7)	-11(4)	0.1986	2316.272	156.528	5
3S	2.18(3)	9(2)					
2S	2.36(7)	15(9)	-10(4)	0.1966	2292.724	154.936	5
5S	2.21(3)	13(2)					
1S	2.45(5)	8(5)	-10(4)	0.1866	2175.558	147.018	5
4S	2.20(3)	11(2)					
2S	2.42(5)	13(6)	-9(4)	0.1812	2112.605	142.764	5
3S	2.36(6)	18(9)					
3S	2.18(3)	9(2)	-10(4)	0.1915	2233.232	150.916	5
6S	2.18(3)	17(2)					
1S	1.31(0.24)	39(49)	-16(5)	0.2177	2538.085	171.517	5
5S	2.22(2)	13(1)					
2S	2.45(4)	12(5)	-8(3)	0.1703	1985.319	134.163	5
4S	2.20(2)	11(2)					
3S	2.42(4)	17(6)	-8(3)	0.1673	1951.261	131.861	5

Ni-N(2.0) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.01(3)	4(2)					5
1S	2.26(4)	6(3)	-3(5)	0.2240	2611.968	176.510	
1N/O	1.97(5)	3(4)					5
2S	2.22(4)	8(2)	-9(5)	0.2409	2809.414	189.853	
2N/O	2.01(4)	5(3)					
2S	2.25(5)	12(4)	-5(5)	0.2191	2554.969	172.658	5
3N/O	2.08(2)	5(1)					
1S	2.64(7)	17(11)	6(2)	0.1636	1908.028	128.940	5
1N/O	1.98(6)	5(6)					
3S	2.21(4)	12(3)	-10(5)	0.2268	2644.498	178.708	5

1N/O 4S			No Fit	No Fit	No Fit	No Fit	5
4N/O 1S	2.08(1) 2.64(5)	7(1) 14(8)	6(2)	0.1207	1407.076	95.087	5
2N/O 3S			No Fit	No Fit	No Fit	No Fit	5
3N/O 2S	2.08(2) 2.63(7)	5(1) 26(12)	6(2)	0.1526	1779.567	120.258	5
5N/O 1S	2.07(2) 1.94(0.12)	9(2) 32(34)	5(2)	0.1397	1628.677	110.062	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.08(1) 2.65(5)	7(1) 22(8)	6(2)	0.1124	1310.334	88.549	5
2N/O 4S			No Fit	No Fit	No Fit	No Fit	5
3N/O 3S	1.94(0.22) 2.19(4)	24(14) 11(3)	-13(9)	0.2220	2588.831	174.946	5
6N/O 1S	2.07(3) 2.00(0.16)	10(2) 21(21)	4(2)	0.1450	1690.903	114.267	5
1N/O 6S	2.69(6) 2.19(2)	4(7) 17(2)	-13(3)	0.1980	2309.300	156.056	5
5N/O 2S	2.08(2) 1.95(7)	9(2) 37(21)	6(2)	0.1337	1558.823	105.341	5
2N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 3S	2.08(1) 2.66(5)	7(1) 27(8)	6(1)	0.1089	1269.518	85.791	5
3N/O 4S			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.07(2)	3(2)	5(4)	0.2600	3031.839	204.884	5

1Br	2.44(6)	15(7)					
1N/O	2.07(3)	0(2)					5
2Br	2.45(7)	18(7)	5(8)	0.4268	4976.476	336.297	
2N/O	2.07(2)	3(2)					
2Br	2.45(7)	21(8)	5(4)	0.2586	3015.871	203.805	5
3N/O	2.07(2)	5(1)					
1Br	2.42(7)	18(9)	5(3)	0.1749	2039.331	137.813	5
1N/O	2.07(3)	0(2)					
3Br	2.46(8)	22(7)	6(8)	0.4248	4953.781	334.764	5
1N/O	2.07(3)	0(2)					
4Br	2.47(8)	25(7)	6(7)	0.4240	4943.881	334.095	5
4N/O	2.08(2)	8(2)					
1Br	2.39(6)	19(9)	4(2)	0.1367	1594.533	107.754	5
2N/O	2.08(2)	3(2)					
3Br	2.45(7)	26(9)	5(4)	0.2582	3010.959	203.473	5
3N/O	2.08(2)	5(2)					
2Br	2.42(7)	24(10)	5(3)	0.1728	2014.423	136.129	5
5N/O	2.08(2)	10(2)					
1Br	2.37(5)	17(7)	4(2)	0.1274	1485.482	100.385	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.08(2)	7(2)					
2Br	2.39(6)	24(9)	5(2)	0.1334	1555.709	105.131	5
2N/O	2.08(2)	3(2)					
4Br	2.46(7)	29(9)	6(4)	0.2583	3011.396	203.502	5
3N/O	2.08(2)	5(2)					
3Br	2.42(6)	28(10)	5(2)	0.1718	2003.291	135.377	5
6N/O	2.09(2)	12(2)					
1Br	2.37(4)	15(5)	4(2)	0.1347	1570.333	106.119	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.09(2)	10(2)					
2Br	2.38(5)	22(7)	4(2)	0.1237	1442.119	97.455	5

2N/O	2.08(2)	3(2)					
5Br	2.46(7)	31(10)	6(4)	0.2585	3014.728	203.727	5
4N/O	2.08(2)	7(1)					
3Br	2.39(5)	28(8)	5(2)	0.1320	1539.373	104.027	5
3N/O	2.08(2)	5(2)					
4Br	2.42(6)	31(10)	5(2)	0.1715	2000.007	135.155	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	7(2)					
1S	4.61(8)	1(7)					
1Br	2.40(7)	19(9)	4(2)	0.1263	1472.292	115.042	7
3N/O	2.06(2)	5(2)					
2S	2.50(9)	23(13)					
1Br	2.44(6)	13(6)	4(3)	0.1259	1468.158	114.719	7
2N/O	2.02(3)	4(2)					
3S	2.37(6)	18(6)					
1Br	2.37(4)	9(3)	0(3)	0.1451	1691.595	132.178	7
1N/O							
4S							
1Br			No Fit	No Fit	No Fit	No Fit	7
3N/O	2.06(2)	4(1)					
1S	2.55(3)	1(3)					
2Br	2.50(3)	9(3)	5(2)	0.1155	1346.230	105.192	7
2N/O	2.07(2)	3(2)					
1S	3.15(8)	9(9)					
3Br	2.47(8)	27(11)	5(4)	0.2350	2740.206	214.115	7
1N/O	1.97(3)	1(3)					
1S	2.23(3)	2(3)					
4Br	2.16(0.12)	32(19)	-6(5)	0.2517	2934.425	229.290	7

Ni-N(2.0) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.08(2)	14(2)					
1Imd	2.06(2)	3(2)	4(2)	0.0901	1050.108	70.964	5
4N/O	2.09(3)	17(4)					
1Imd	1.99(2)	0(3)					
1Imd	2.12(2)	0(3)	3(1)	0.0692	807.378	63.087	7
3N/O	2.08(2)	9(3)	1(1)	0.0550	641.805	59.438	9

1Imd	1.87(4)	3(5)					
1Imd	2.11(2)	3(3)					
1Imd	1.98(2)	3(3)					
2N/O	2.08(2)	5(3)					
1Imd	1.89(9)	3(10)					
1Imd	1.99(4)	3(5)					
1Imd	1.96(0.66)	29(110)					
1Imd	2.12(4)	2(4)	1(3)	0.0562	655.695	74.529	11
1N/O	2.08(3)	1(4)					
1Imd	2.76(0.19)	14(23)					
1Imd	1.86(5)	2(7)					
1Imd	1.96(5)	8(6)					
1Imd	2.08(6)	9(6)					
1Imd	2.19(5)	6(7)	1(2)	0.0637	742.643	109.247	13
4N/O	2.08(2)	11(2)					
1Imd	2.06(3)	4(3)	4(2)	0.0853	995.101	67.246	5
3N/O	2.08(2)	10(3)					
1Imd	2.11(3)	1(3)					
1Imd	1.99(3)	2(3)	3(1)	0.0649	756.919	59.144	7
2N/O	2.08(2)	5(3)					
1Imd	2.13(2)	3(3)					
1Imd	2.00(2)	3(3)					
1Imd	1.90(4)	2(5)	1(1)	0.0571	665.358	61.619	9
1N/O	2.08(3)	1(3)					
1Imd	2.19(4)	6(6)					
1Imd	1.97(4)	9(5)					
1Imd	1.86(4)	3(6)					
1Imd	2.08(4)	9(5)	1(2)	0.0673	784.956	89.221	11
0N/O							
1Imd	2.21(0.47)	4(104)					
1Imd	2.18(0.24)	8(22)					
1Imd	1.97(0.10)	11(11)					
1Imd	2.08(0.16)	12(13)					
1Imd	1.87(5)	6(10)	2(2)	0.1277	1488.697	169.211	11
3N/O	2.08(2)	8(3)					
1Imd	2.05(3)	4(4)	4(2)	0.0963	1122.777	75.874	5
2N/O	2.08(2)	5(3)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(2)	0(2)	4(1)	0.0722	842.386	65.822	7
1N/O	2.07(3)	1(3)	2(2)	0.0773	901.836	83.520	9

1Imd	1.92(4)	0(6)					
1Imd	2.03(3)	4(4)					
1Imd	2.15(3)	3(3)					
0N/O							
1Imd	1.98(2)	12(4)					
1Imd	2.21(3)	9(4)					
1Imd	2.10(2)	13(4)					
1Imd	1.88(3)	6(4)	2(2)	0.1312	1529.996	141.695	9
2N/O	2.08(3)	5(3)					
1Imd	2.05(4)	4(4)	4(2)	0.1413	1647.880	111.359	5
1N/O	2.08(3)	1(3)					
1Imd	2.13(3)	1(2)					
1Imd	1.99(2)	1(2)	4(2)	0.1115	1300.714	101.635	7
0N/O							
1Imd	1.94(3)	3(6)					
1Imd	2.04(3)	6(5)					
1Imd	2.16(3)	5(4)	3(2)	0.1645	1918.242	149.888	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(3)	13(5)					
1S	1.88(0.10)	33(32)					
1Imd	2.07(3)	3(3)	5(2)	0.0794	926.399	72.387	7
3N/O	2.08(2)	10(3)					
1S	2.61(3)	14(5)					
1Imd	2.14(2)	1(3)					
1Imd	2.01(2)	1(2)	5(1)	0.0414	482.580	44.692	9
2N/O							
1S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(3)	13(5)					
1S	1.88(0.10)	32(31)					
1Imd	2.07(2)	3(3)	5(2)	0.0781	911.099	71.192	7
3N/O	2.08(2)	10(3)					
1S	2.62(3)	14(5)					
1Imd	2.14(2)	1(3)					
1Imd	2.01(2)	1(2)	4(1)	0.0406	473.340	43.836	9

2N/O	2.07(2)	5(3)					
1S	2.55(8)	21(12)					
1Imd	2.01(3)	3(4)					
1Imd	2.14(3)	2(3)					
1Imd	1.91(5)	3(7)	2(2)	0.0436	508.531	57.802	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	11(2)					
1S	2.65(4)	14(5)					
1Imd	2.07(2)	4(3)	5(1)	0.0550	641.509	50.126	7
3N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O	2.07(2)	5(3)					
1S	2.56(8)	21(11)					
1Imd	2.14(3)	3(3)					
1Imd	1.91(5)	3(6)					
1Imd	2.01(3)	3(4)	2(2)	0.0419	488.112	55.481	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	11(2)					
1S	2.66(4)	14(5)					
1Imd	2.07(2)	4(3)	5(1)	0.0549	640.053	50.013	7
3N/O	2.07(2)	10(3)					
1S	2.63(3)	15(5)					
1Imd	2.14(2)	0(2)					
1Imd	2.01(2)	1(2)	4(1)	0.0402	468.419	43.381	9
2N/O	2.07(2)	5(3)					
1S	2.56(8)	22(12)					
1Imd	2.01(3)	3(3)					
1Imd	1.90(5)	2(6)					
1Imd	2.14(3)	3(3)	2(2)	0.0414	482.186	54.807	11

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.10(2)	12(3)					
1Br	2.38(4)	17(5)					
1Imd	2.06(2)	4(3)	4(1)	0.0677	789.575	61.696	7
3N/O	2.10(2)	11(4)					
1Br	2.35(4)	17(6)					
1Imd	2.00(2)	1(3)	4(1)	0.0507	590.930	54.727	9

1Imd	2.13(3)	1(3)					
2N/O	2.08(3)	5(3)					
1Br	2.28(0.13)	24(16)					
1Imd	1.91(6)	2(7)					
1Imd	2.14(3)	2(4)					
1Imd	2.01(4)	3(5)	2(2)	0.0516	602.132	68.441	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(2)	12(3)					
1Br	2.38(4)	17(5)					
1Imd	2.06(2)	4(3)	4(1)	0.0670	781.845	61.092	7
3N/O	2.09(2)	11(4)					
1Br	2.36(4)	18(5)					
1Imd	2.00(2)	1(3)					
1Imd	2.13(3)	1(3)	4(1)	0.0501	584.721	54.152	9
2N/O	2.08(3)	5(3)					
1Br	2.29(0.12)	24(15)					
1Imd	2.14(3)	2(4)					
1Imd	2.01(4)	3(5)					
1Imd	1.92(6)	3(8)	2(2)	0.0512	597.341	67.896	11

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(2)	12(3)					
1Br	2.39(4)	17(5)					
1Imd	2.06(2)	4(3)	4(1)	0.0665	775.732	60.614	7
3N/O	2.09(2)	11(4)					
1Br	2.36(4)	18(5)					
1Imd	2.00(2)	1(3)					
1Imd	2.13(3)	1(3)	4(1)	0.0497	579.859	53.701	9
2N/O	2.08(3)	5(3)					
1Br	2.30(0.11)	24(15)					
1Imd	2.14(3)	2(4)					
1Imd	1.92(6)	3(8)					
1Imd	2.01(4)	2(5)	2(2)	0.0509	593.331	67.440	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	11(2)					
1Br	2.85(4)	15(6)					
1Imd	2.07(2)	3(3)	4(2)	0.0695	810.145	63.303	7
3N/O			No Fit	No Fit	No Fit	No Fit	9

1Br							
1Imd							
1Imd							
2N/O	2.07(3)	7(4)					
1Br	2.82(5)	16(7)					
1Imd	2.01(3)	3(3)					
1Imd	1.91(5)	4(8)					
1Imd	2.14(2)	3(3)	2(2)	0.0468	545.461	61.999	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	7(2)					
2S	2.63(5)	24(7)					
1Imd	2.08(3)	5(4)	6(1)	0.0670	780.903	61.018	7
2N/O	2.07(2)	6(3)					
2S	2.59(5)	25(7)					
1Imd	2.00(2)	0(2)					
1Imd	2.14(2)	0(2)	5(1)	0.0462	538.992	49.917	9
1N/O	2.06(3)	1(3)					
2S	2.45(8)	29(11)					
1Imd	1.90(4)	0(4)					
1Imd	2.14(2)	4(2)					
1Imd	2.01(3)	5(3)	1(2)	0.0474	552.386	62.786	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	8(2)					
2S	2.64(5)	24(7)					
1Imd	2.08(3)	5(4)	5(1)	0.0658	767.788	59.993	7
2N/O	2.07(2)	6(3)					
2S	2.60(5)	26(8)					
1Imd	2.14(2)	0(2)					
1Imd	2.00(2)	0(2)	5(1)	0.0456	531.673	49.239	9
1N/O	2.06(2)	1(3)					
2S	2.47(8)	30(11)					
1Imd	2.14(2)	4(2)					
1Imd	1.90(3)	0(4)					
1Imd	2.01(3)	5(3)	1(2)	0.0466	542.915	61.710	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	8(2)					
2S	2.65(5)	26(8)					
1Imd	2.08(3)	5(4)	5(1)	0.0655	764.335	59.724	7

2N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	8(2)					
2S	2.65(5)	26(8)					
1Imd	2.07(3)	5(4)	5(1)	0.0659	767.979	60.008	7
2N/O	2.07(2)	6(3)					
2S	2.61(5)	28(9)					
1Imd	2.14(2)	0(2)					
1Imd	2.00(2)	0(2)	4(1)	0.0469	547.257	50.682	9
1N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(2)	8(3)					
2Br	2.38(5)	25(8)					
1Imd	2.06(3)	4(4)	5(2)	0.0831	968.530	75.679	7
2N/O	2.09(2)	5(3)					
2Br	2.33(6)	26(9)					
1Imd	2.00(2)	0(2)					
1Imd	2.14(3)	0(2)	4(1)	0.0608	709.021	65.663	9
1N/O	2.07(3)	1(3)					
2Br	2.23(0.17)	33(21)					
1Imd	1.92(4)	2(5)					
1Imd	2.03(4)	5(4)					
1Imd	2.15(3)	4(4)	2(2)	0.0701	817.164	92.882	11

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(2)	8(3)	5(2)	0.0818	954.045	74.547	7

2Br	2.39(5)	25(8)					
1Imd	2.06(3)	4(4)					
2N/O	2.09(2)	5(3)					
2Br	2.34(6)	26(9)					
1Imd	2.14(2)	0(2)					
1Imd	2.00(2)	0(2)	4(1)	0.0598	697.762	64.620	9
1N/O	2.07(3)	1(3)					
2Br	2.25(0.15)	32(20)					
1Imd	2.03(4)	5(4)					
1Imd	1.92(4)	2(5)					
1Imd	2.15(3)	4(4)	2(2)	0.0682	807.368	91.769	11

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(2)	8(3)					
2Br	2.39(5)	25(7)					
1Imd	2.06(3)	4(4)	5(2)	0.0684	797.578	90.656	7
2N/O	2.09(2)	5(3)					
2Br	2.35(6)	26(8)					
1Imd	2.14(2)	0(2)					
1Imd	2.00(2)	0(2)	4(1)	0.0590	687.772	63.695	9
1N/O	2.07(3)	1(3)					
2Br	2.27(0.14)	3(4)					
1Imd	2.03(4)	5(5)					
1Imd	2.16(3)	4(4)					
1Imd	1.93(4)	2(5)	2(2)	0.0807	941.073	73.534	11

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(2)	7(3)					
2Br	3.35(9)	21(11)					
1Imd	2.06(5)	5(5)	4(2)	0.0819	954.644	74.594	7
2N/O	2.07(3)	7(4)					
2Br	2.83(4)	20(6)					
1Imd	2.14(2)	1(2)					
1Imd	2.00(2)	0(2)	4(1)	0.0604	704.176	65.214	9
1N/O	2.07(3)	2(4)					
2Br	2.82(6)	22(9)					
1Imd	2.16(3)	3(4)					
1Imd	1.94(5)	1(8)					
1Imd	2.03(4)	3(6)	3(2)	0.0686	800.044	90.936	11

Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(0.22)	45(83)					
1N/O	2.10(4)	3(4)					
1S	1.77(0.12)	28(14)					
1Imd	2.13(3)	0(3)					
1Imd	1.99(2)	0(2)	4(2)	0.0518	604.580	68.719	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(6)	14(9)					
1N/O	2.11(5)	4(4)					
1S	2.62(4)	15(5)					
1Imd	2.13(2)	0(3)					
1Imd	2.00(2)	0(2)	3(1)	0.0345	407.623	46.332	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(9)	13(17)					
2N/O	2.11(3)	6(4)					
1S	2.62(4)	14(5)					
1Imd	2.12(2)	0(3)					
1Imd	1.99(2)	0(2)	3(1)	0.0332	387.201	44.011	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(6)	10(10)					
2N/O	2.12(2)	6(4)					
1S	2.62(4)	15(5)					
1Imd 0°	2.12(2)	1(2)					
1Imd 5°	1.99(2)	1(2)	3(1)	0.0339	350.453	39.834	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(6)	5(5)					
2N/O	2.11(4)	8(8)					
1S	2.63(5)	16(6)					
1Imd 0°	2.06(4)	4(3)					
1Imd 10°	2.11(5)	4(5)	3(1)	0.0368	429.650	48.836	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.98(7)	4(5)					
2N/O	2.10(5)	11(10)					
1S	2.63(5)	15(7)					
1Imd 5°	2.07(4)	4(4)					
1Imd 10°	2.12(4)	3(4)	4(1)	0.0411	479.438	54.495	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(0.11)	11(18)					
2N/O	2.10(4)	8(7)					
1S	2.62(4)	15(6)					
1Imd 5°	2.00(2)	1(2)					
1Imd 5°	2.13(2)	1(3)	3(1)	0.0399	465.245	52.882	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.10(3)	1(5)					
2N/O	1.96(4)	5(5)					
1S	2.56(8)	19(10)					
1Imd 10°	2.15(3)	4(2)					
1Imd 10°	2.02(3)	3(3)	1(2)	0.0437	509.232	57.881	11

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(3)	6(4)					
1Br	2.38(6)	10(4)					
1Br	2.17(7)	11(7)					
1Imd	2.05(4)	4(4)	3(2)	0.0780	909.778	84.255	9
2N/O	2.06(3)	0(4)					
1Br	2.16(5)	6(5)					
1Br	2.36(5)	8(4)					
1Imd	2.11(3)	1(2)					
1Imd	1.97(3)	1(2)	2(2)	0.0466	543.489	61.775	11
1N/O	2.03(4)	6(5)					
1Br	2.13(5)	2(6)					
1Br	2.33(5)	6(6)					
1Imd	2.01(0.21)	12(29)					
1Imd	1.95(5)	3(5)					
1Imd	2.11(5)	4(4)	1(2)	0.0492	573.652	84.387	13

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(3)	6(4)					
1Br	2.15(7)	10(6)					
1Br	2.37(5)	11(4)					
1Imd	2.04(4)	3(4)	3(2)	0.0762	888.281	82.265	9

2N/O	2.06(3)	0(4)					
1Br	2.16(5)	7(5)					
1Br	2.36(5)	9(4)					
1Imd	1.97(3)	1(2)					
1Imd	2.11(3)	1(2)	2(2)	0.0463	539.859	61.363	11
1N/O	2.03(4)	6(5)					
1Br	2.13(5)	3(6)					
1Br	2.33(5)	6(6)					
1Imd	2.00(0.20)	11(29)					
1Imd	1.95(6)	3(6)					
1Imd	2.11(6)	4(4)	1(2)	0.0487	567.542	83.488	13

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(3)	7(4)					
1Br	2.41(6)	11(6)					
1Br	2.22(0.11)	14(10)					
1Imd	2.06(4)	4(4)	4(2)	0.0779	907.913	84.083	9
2N/O	2.07(3)	1(4)					
1Br	2.37(5)	8(4)					
1Br	2.18(5)	7(6)					
1Imd	1.97(3)	1(2)					
1Imd	2.11(3)	1(2)	3(2)	0.0481	560.355	63.692	11
1N/O	2.06(4)	1(5)					
1Br	2.17(0.11)	19(13)					
1Br	2.80(7)	14(8)					
1Imd	2.02(4)	5(4)					
1Imd	2.14(4)	5(3)					
1Imd	1.92(5)	1(6)	2(2)	0.0605	704.946	103.701	13

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(3)	7(4)					
1Br	2.42(7)	12(7)					
1Br	2.24(0.12)	15(12)					
1Imd	2.06(4)	4(4)	4(2)	0.0780	909.115	84.194	9
2N/O	2.07(3)	6(4)					
1Br	2.34(7)	21(9)					
1Br	3.27(6)	12(7)					
1Imd	2.15(3)	1(2)					
1Imd	2.01(3)	0(2)	4(1)	0.0525	612.761	69.649	11
1N/O	2.06(4)	1(5)					
1Br	2.17(0.11)	19(14)					
1Br	2.80(7)	14(8)					
1Imd	2.14(4)	5(3)	2(2)	0.0612	713.059	104.895	13

1Imd	1.92(5)	1(6)					
1Imd	2.02(4)	5(4)					

Ni-N(2.0) Ni-Br(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(3)	8(3)					
1Br	2.88(7)	15(8)					
1Br	2.36(8)	21(12)					
1Imd	2.08(4)	4(5)	5(2)	0.0762	888.871	82.319	9
2N/O	2.07(3)	6(4)					
1Br	2.30(8)	22(12)					
1Br	2.85(6)	14(7)					
1Imd	2.15(3)	1(3)					
1Imd	2.01(3)	1(3)	4(1)	0.0528	615.743	69.988	11
1N/O	2.06(4)	1(4)					
1Br	2.19(0.12)	20(15)					
1Br	2.81(7)	14(8)					
1Imd	2.15(4)	5(3)					
1Imd	1.92(5)	1(6)					
1Imd	2.02(4)	5(4)	2(2)	0.0610	711.260	104.630	13

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	7(2)					
1S	2.52(2)	5(2)					
1Br	2.48(2)	1(2)					
1Imd	2.08(2)	0(2)	4(1)	0.0407	475.109	44.000	9
2N/O	2.05(3)	6(4)					
1S	2.50(5)	1(10)					
1Br	2.45(5)	5(9)					
1Imd	2.12(3)	0(3)					
1Imd	2.00(3)	1(3)	4(1)	0.0404	471.620	53.606	11
1N/O	2.06(3)	1(3)					
1S	2.40(6)	1(6)					
1Br	2.36(6)	6(6)					
1Imd	2.11(3)	4(3)					
1Imd	1.88(4)	2(5)					
1Imd	1.98(3)	4(3)	0(2)	0.0349	407.074	59.883	13

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	7(2)					
1S	2.53(2)	5(2)					
1Br	2.48(2)	1(2)					
1Imd	2.08(2)	0(2)	5(1)	0.0414	482.556	44.690	9

2N/O	2.05(3)	7(4)					
1S	2.49(6)	3(10)					
1Br	2.44(5)	7(8)					
1Imd	2.13(3)	0(2)					
1Imd	2.00(3)	1(3)	4(1)	0.0405	472.131	53.664	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	7(2)					
1S	2.54(2)	4(2)					
1Br	2.49(2)	0(2)					
1Imd	2.08(2)	1(2)	5(1)	0.0437	509.364	47.173	9
2N/O	2.05(3)	7(4)					
1S	2.48(6)	5(10)					
1Br	2.43(5)	9(8)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(1)	0.0406	473.911	53.867	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	7(3)					
1S	2.59(6)	16(9)					
1Br	2.89(5)	13(6)					
1Imd	2.10(4)	4(5)	5(2)	0.0628	732.589	67.846	9
2N/O	2.06(3)	7(4)					
1S	2.55(6)	17(9)					
1Br	2.85(5)	13(5)					
1Imd	2.15(2)	1(2)					
1Imd	2.01(2)	1(3)	4(1)	0.0405	472.443	53.700	11
1N/O	2.05(4)	3(5)					
1S	2.41(7)	15(9)					
1Br	2.81(5)	13(6)	1(2)	0.0412	480.989	70.756	13

1Imd	2.00(3)	5(3)					
1Imd	1.90(4)	1(5)					
1Imd	2.13(3)	5(2)					

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.3) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(1)	7(2)					
1S	2.52(2)	5(2)					
1Br	2.47(2)	1(2)					
1Imd	2.07(2)	0(2)	4(1)	0.0432	503.717	46.651	9
2N/O	2.05(3)	7(4)					
1S	2.50(6)	3(12)					
1Br	2.44(6)	7(10)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(1)	0.0408	476.125	54.118	11
1N/O	2.05(3)	2(3)					
1S	2.41(6)	1(6)					
1Br	2.37(6)	5(6)					
1Imd	1.88(4)	2(5)					
1Imd	2.11(3)	4(3)					
1Imd	1.98(3)	4(3)	0(2)	0.0342	398.520	58.624	13

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(1)	7(2)					
1S	2.53(2)	6(2)					
1Br	2.48(2)	1(2)					
1Imd	2.08(2)	0(2)	4(1)	0.0417	486.169	45.025	9
2N/O	2.05(3)	7(4)					
1S	2.50(6)	4(11)					
1Br	2.44(6)	8(9)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(1)	0.0406	473.904	53.866	11
1N/O	2.05(3)	1(3)					
1S	2.41(6)	2(6)					
1Br	2.37(6)	6(5)					
1Imd	1.98(3)	4(3)					
1Imd	1.88(4)	2(5)					
1Imd	2.11(3)	4(3)	0(2)	0.0339	395.494	58.179	13

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	7(2)					
1S	2.53(2)	5(2)					
1Br	2.49(2)	1(2)	4(1)	0.0427	498.480	46.165	9

1Imd	2.08(2)	0(2)					
2N/O	2.05(3)	7(4)					
1S	2.49(6)	6(11)					
1Br	2.44(6)	9(8)					
1Imd	1.99(3)	1(3)					
1Imd	2.12(3)	0(2)	3(1)	0.0407	474.452	53.928	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	7(3)					
1S	2.59(6)	16(9)					
1Br	2.89(5)	13(6)					
1Imd	2.10(4)	4(5)	5(2)	0.0623	725.887	67.225	9
2N/O	2.06(3)	7(4)					
1S	2.56(6)	18(10)					
1Br	2.86(5)	14(6)					
1Imd	2.01(2)	1(3)					
1Imd	2.15(2)	1(2)	4(1)	0.0403	470.189	53.444	11
1N/O	2.05(4)	3(5)					
1S	2.42(7)	16(10)					
1Br	2.81(5)	13(6)					
1Imd	1.90(4)	1(5)					
1Imd	2.01(3)	5(3)					
1Imd	2.13(3)	5(2)	1(2)	0.0412	480.886	70.741	13

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.3) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.03(2)	8(2)					
1S	2.51(2)	6(2)					
1Br	2.46(2)	2(2)					
1Imd	2.07(2)	1(2)	3(1)	0.0455	530.684	49.147	9
2N/O	2.05(3)	7(4)					
1S	2.51(7)	5(12)					
1Br	2.44(6)	8(10)					
1Imd	1.99(3)	1(3)					
1Imd	2.12(3)	0(2)	3(2)	0.0411	479.088	54.455	11
1N/O	2.05(3)	1(3)					
1S	2.43(6)	0(7)	0(2)	0.0335	390.664	57.469	13

1Br	2.38(5)	4(6)					
1Imd	1.98(3)	4(3)					
1Imd	1.88(4)	2(5)					
1Imd	2.11(3)	4(3)					

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(1)	7(2)					
1S	2.52(2)	6(2)					
1Br	2.47(2)	2(2)					
1Imd	2.07(2)	1(2)	4(1)	0.0426	497.139	46.041	9
2N/O	2.05(3)	7(4)					
1S	2.50(6)	5(12)					
1Br	2.44(6)	8(9)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(1)	0.0409	476.353	54.144	11
1N/O	2.05(3)	1(3)					
1S	2.42(6)	1(6)					
1Br	2.38(5)	5(6)					
1Imd	1.98(3)	4(3)					
1Imd	1.88(4)	2(5)					
1Imd	2.11(3)	4(3)	0(2)	0.0334	389.031	57.229	13

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(1)	7(2)					
1S	2.53(2)	6(2)					
1Br	2.48(2)	1(2)					
1Imd	2.08(2)	1(2)	4(1)	0.0428	498.778	46.192	9
2N/O	2.05(3)	7(4)					
1S	2.50(6)	6(11)					
1Br	2.44(6)	9(8)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(1)	0.0409	476.457	54.156	11
1N/O	2.05(3)	1(3)					
1S	2.42(6)	2(6)					
1Br	2.38(5)	6(5)					
1Imd	1.88(4)	2(5)					
1Imd	2.11(3)	4(3)					
1Imd	1.98(3)	4(3)	0(2)	0.0331	386.005	56.783	13

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(1)	7(2)					
1S	2.53(2)	5(2)	4(1)	0.0446	519.768	48.136	9

1Br	2.48(2)	1(2)					
1Imd	2.08(2)	0(2)					
2N/O	2.05(3)	7(4)					
1S	2.56(6)	18(10)					
1Br	2.85(5)	14(6)					
1Imd	2.15(2)	1(2)					
1Imd	2.01(2)	1(3)	4(1)	0.0405	472.176	53.670	11
1N/O	2.05(4)	3(5)					
1S	2.43(7)	17(10)					
1Br	2.82(5)	13(6)					
1Imd	2.01(3)	5(3)					
1Imd	2.13(3)	5(2)					
1Imd	1.90(4)	1(4)	1(2)	0.0412	480.680	70.711	13

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(3)	8(4)					
1S	2.54(9)	8(14)					
1Br	2.46(0.11)	11(9)					
1Imd	2.07(3)	4(3)	4(2)	0.0599	698.350	64.675	9
2N/O	2.05(3)	7(4)					
1S	2.51(7)	6(12)					
1Br	2.44(7)	9(9)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(2)	0.0412	480.944	54.666	11
1N/O	2.05(3)	1(3)					
1S	2.44(5)	0(7)					
1Br	2.39(5)	3(6)					
1Imd	2.11(3)	4(3)					
1Imd	1.98(3)	4(3)					
1Imd	1.88(4)	2(5)	0(2)	0.0327	381.864	56.174	13

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.03(2)	8(2)					
1S	2.52(2)	6(2)					
1Br	2.46(2)	2(2)					
1Imd	2.07(2)	0(2)	3(1)	0.0448	522.834	48.420	9
2N/O	2.05(3)	7(4)					
1S	2.51(6)	6(12)					
1Br	2.44(6)	9(9)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(2)	0.0410	478.644	54.405	11
1N/O	2.05(3)	1(3)	0(2)	0.0328	382.060	56.203	13

1S	2.43(6)	1(7)					
1Br	2.39(5)	5(6)					
1Imd	1.98(3)	4(3)					
1Imd	1.88(4)	2(5)					
1Imd	2.11(3)	4(3)					

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(1)	8(2)					
1S	2.52(2)	6(2)					
1Br	2.47(2)	1(2)					
1Imd	2.07(2)	1(2)	3(1)	0.0413	481.801	54.764	9
2N/O	2.04(2)	5(3)					
1S	2.52(4)	4(4)					
1Br	2.47(4)	0(4)					
1Imd	2.00(6)	7(13)					
1Imd	2.09(6)	1(3)	3(1)	0.0442	515.214	47.714	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(1)	7(2)					
1S	2.53(2)	6(2)					
1Br	2.48(2)	1(2)					
1Imd	2.08(2)	0(2)	4(1)	0.0455	530.736	49.152	9
2N/O	2.05(3)	7(4)					
1S	2.50(7)	8(11)					
1Br	2.44(6)	10(8)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(2)	0.0413	481.168	54.692	11
1N/O	2.05(2)	1(3)					
1S	2.42(5)	2(6)					
1Br	2.38(5)	5(5)					
1Imd	1.88(4)	2(5)					
1Imd	1.98(3)	4(3)					
1Imd	2.11(3)	4(3)	0(2)	0.0324	377.897	55.591	13

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.3) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(3)	8(4)	4(2)	0.0603	702.708	65.079	9

1S	2.55(9)	10(15)					
1Br	2.46(0.11)	12(8)					
1Imd	2.06(3)	4(3)					
2N/O	2.06(3)	7(4)					
1S	2.52(7)	6(12)					
1Br	2.45(7)	9(9)					
1Imd	1.98(3)	1(3)					
1Imd	2.11(3)	0(2)	3(2)	0.0413	481.795	54.763	11
1N/O	2.04(3)	1(3)					
1S	2.44(5)	0(7)					
1Br	2.39(5)	3(6)					
1Imd	1.88(4)	2(5)					
1Imd	2.11(2)	4(3)					
1Imd	1.98(3)	4(3)	0(2)	0.0322	375.792	55.281	13

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.4) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(3)	8(3)					
1S	2.55(9)	10(15)					
1Br	2.46(0.10)	12(9)					
1Imd	2.07(3)	4(3)	4(2)	0.0601	700.383	64.863	9
2N/O	2.05(3)	7(4)					
1S	2.51(7)	6(12)					
1Br	2.45(6)	9(9)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(2)	0.0412	480.044	54.564	11
1N/O	2.05(2)	1(3)					
1S	2.44(5)	1(7)					
1Br	2.39(5)	5(6)					
1Imd	1.98(3)	4(3)					
1Imd	2.11(2)	4(3)					
1Imd	1.88(4)	2(5)	0(2)	0.0323	376.629	55.404	13

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.5) Ni-Imid

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(3)	8(3)					
1S	2.55(8)	10(15)					
1Br	2.46(0.10)	12(9)					
1Imd	2.07(3)	4(3)	4(2)	0.0600	699.479	64.779	9
2N/O	2.05(3)	7(4)					
1S	2.51(7)	7(12)					
1Br	2.45(6)	10(8)					
1Imd	2.12(3)	0(2)					
1Imd	1.99(3)	1(3)	3(2)	0.0412	480.734	54.642	11

1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(3)	8(3)					
1S	2.54(8)	11(16)					
1Br	2.46(9)	13(9)					
1Imd	2.07(3)	4(3)	4(2)	0.0601	701.058	64.926	9
2N/O	2.05(3)	7(4)					
1S	2.5(7)	8(11)					
1Br	2.44(6)	10(8)					
1Imd 0°	2.12(3)	0(2)					
1Imd 0°	1.99(3)	1(3)	3(2)	0.0415	483.515	54.958	11
2N/O	2.05(4)	9(6)					
1S	2.52(7)	8(13)					
1Br	2.46(7)	10(10)					
1Imd 0°	2.13(3)	1(3)					
1Imd 5°	2.00(2)	1(3)	3(2)	0.0437	451.689	51.341	11
2N/O	2.03(2)	4(3)					
1S	2.62(6)	19(9)					
1Br	3.31(0.11)	18(15)					
1Imd 0°	2.08(6)	6(6)					
1Imd 10°	2.14(3)	2(3)	4(1)	0.0471	549.335	62.440	11
2N/O	2.02(3)	4(3)					
1S	2.60(0.11)	24(17)					
1Br	2.82(9)	18(12)					
1Imd 5°	2.07(5)	3(5)					
1Imd 10°	2.15(3)	1(2)	4(2)	0.0526	613.279	69.708	11
1N/O	2.05(2)	1(3)					
1S	2.43(5)	2(6)					
1Br	2.39(5)	6(5)					
1Imd	1.87(4)	2(5)					
1Imd	2.11(3)	4(3)					
1Imd	1.98(3)	4(3)	0(2)	0.0321	373.822	54.991	13

Ni-N(2.0) Ni-N(2.2) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(6)	6(7)					
1N/O	2.09(3)	0(3)	2(2)	0.0323	376.916	55.446	9

1S	2.50(6)	1(8)					
1Br	2.45(5)	4(7)					
1Imd 0°	2.12(3)	2(2)					
1Imd 5°	1.99(2)	2(2)					
1N/O	1.96(4)	3(5)					
1N/O	2.10(6)	2(8)					
1S	2.50(8)	8(17)					
1Br	2.44(8)	11(13)					
1Imd 0°	2.04(4)	3(4)					
1Imd 10°	2.10(6)	4(6)	2(2)	0.0385	448.411	65.964	9
1N/O	1.96(5)	2(6)					
1N/O	2.09(8)	3(11)					
1S	2.51(9)	8(18)					
1Br	2.44(8)	11(14)					
1Imd 5°	2.05(4)	3(4)					
1Imd 10°	2.11(5)	3(5)	2(2)	0.0430	501.602	73.788	9

Table G.3. Additional Fits for Co(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(3)	2(2)	neg2(7)	0.2866	1399.137	205.850	3
3N/O	2.09(3)	4(2)	neg2(4)	0.1835	895.611	131.768	3
4N/O	2.09(2)	6(2)	neg2(3)	0.1320	644.145	94.771	3
5N/O	2.09(2)	8(2)	neg2(3)	0.1124	548.519	80.702	3
6N/O	2.09(2)	10(2)	neg3(3)	0.1126	549.592	80.860	3
7N/O	2.10(2)	12(2)	neg3(3)	0.1247	608.851	89.578	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.18(4)	7(2)	neg24(10)	0.2892	1411.525	207.673	3
3S	2.19(4)	10(2)	neg23(7)	0.2196	1071.980	157.717	3
4S	2.20(4)	12(2)	neg22(6)	0.1870	912.846	134.304	3
5S	2.20(4)	14(2)	neg22(6)	0.1736	847.526	124.693	3
6S	2.20(4)	16(2)	neg22(6)	0.1708	833.597	122.644	3
7S	2.20(4)	17(2)	neg22(6)	0.1738	848.489	124.835	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.06(3)	1(2)					
1N/O	2.21(3)	3(3)	neg1(4)	0.1185	578.626	120.626	5
2N/O	2.05(2)	1(2)					
2N/O	2.19(3)	2(3)	neg1(3)	0.0927	452.584	94.350	5

3N/O	2.07(2)	2(2)					
1N/O	2.22(4)	1(3)	neg1(3)	0.0909	443.548	92.466	5
4N/O	2.08(2)	5(2)					
1N/O	2.24(4)	1(3)	neg1(3)	0.0907	442.708	92.291	5
3N/O	2.06(3)	3(2)					
2N/O	2.20(4)	4(5)	neg1(3)	0.0940	458.971	95.681	5
5N/O	2.08(3)	7(2)					
1N/O	2.25(7)	3(6)	neg2(3)	0.1045	510.128	106.346	5
4N/O	2.07(3)	6(4)					
2N/O	2.22(0.10)	9(13)	neg2(4)	0.1070	522.480	108.921	5
3N/O	2.07(4)	6(3)					
3N/O	2.18(0.11)	14(14)	neg2(4)	0.1074	524.205	109.281	5
6N/O	2.10(3)	10(2)					
1N/O	2.41(0.20)	16(39)	neg1(4)	0.1095	534.487	111.424	5
5N/O	2.10(3)	8(2)					
2N/O	2.32(0.21)	27(53)	neg1(5)	0.1083	528.806	110.240	5
4N/O	2.09(3)	7(2)					
3N/O	2.24(0.25)	30(35)	neg1(6)	0.1103	538.419	112.244	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.17(4)	4(2)					
1S	2.32(5)	2(3)	neg19(7)	0.1625	793.257	165.370	5
2S	2.16(4)	5(3)					
2S	2.31(5)	6(4)	neg18(7)	0.1495	729.493	152.077	5
3S	2.18(4)	7(2)					
1S	2.34(5)	3(3)	neg19(6)	0.1495	729.724	152.125	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.17(4)	8(3)					
2S	2.33(7)	8(5)	neg19(7)	0.1491	727.971	151.759	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.22(2)	12(2)	neg18(4)	0.0845	412.409	85.974	5

2S	2.97(4)	7(4)					
3S	2.33(8)	12(8)					
3S	2.17(5)	9(4)	neg18(7)	0.1518	740.819	154.438	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.22(2)	14(1)					
2S	2.97(3)	7(3)	neg19(3)	0.0664	324.124	67.570	5
4S	2.20(4)	11(4)					
3S	2.38(0.11)	18(15)	neg17(7)	0.1463	714.267	148.903	5

Co-N(2.0) Co-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.04(3)	2(2)					5
1S	2.32(5)	5(4)	neg7(6)	0.1498	731.378	152.470	
1N/O	2.01(4)	1(3)					5
2S	2.28(6)	9(4)	neg12(8)	0.1728	843.374	175.817	
2N/O	2.48(6)	2(3)					
2S	2.16(4)	6(2)	neg26(7)	0.1746	852.475	177.715	5
3N/O	2.05(3)	4(2)					
1S	2.33(6)	8(5)	neg6(5)	0.1280	624.734	130.238	5
1N/O	1.43(0.15)	12(17)					
3S	2.19(5)	10(2)	neg22(10)	0.2120	1034.938	215.753	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(2)	7(2)					
1S	2.68(4)	7(5)	1(3)	0.1009	492.501	102.671	5
2N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.06(4)	5(2)					
2S	2.33(9)	17(9)	neg7(6)	0.1343	655.721	136.697	5
5N/O	2.10(3)	9(4)					
1S	1.91(0.10)	24(29)	neg1(4)	0.1039	507.158	105.727	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5

4N/O	2.10(2)	6(2)					
2S	2.61(0.11)	27(19)	neg1(3)	0.1044	509.663	106.249	5
2N/O	1.91(0.53)	24(49)					
4S	2.20(6)	12(4)	neg22(14)	0.1774	865.769	180.486	5
3N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
6N/O	2.09(4)	10(4)					
1S	1.96(0.15)	20(30)	neg1(3)	0.1056	515.610	107.489	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.11(2)	8(2)					
2S	2.66(5)	18(8)	1(2)	0.0815	397.986	82.968	5
2N/O	2.78(5)	3(5)					
5S	2.23(4)	14(2)	neg17(6)	0.1371	669.046	139.475	5
4N/O	2.10(2)	6(2)					
3S	2.60(0.11)	33(19)	neg1(3)	0.0989	482.806	100.650	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Table G.4. Additional Fits for Co(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	2(2)	-1(5)	0.3208	1672.059	99.540	3
3N/O	2.10(2)	5(1)	-1(3)	0.2245	1170.183	69.663	3
4N/O	2.10(2)	7(1)	-1(2)	0.1779	927.112	55.192	3
5N/O	2.10(2)	8(1)	-2(2)	0.1618	843.009	50.186	3
6N/O	2.10(2)	10(1)	-2(2)	0.1644	856.578	50.993	3
7N/O	2.10(2)	12(1)	-3(2)	0.1780	927.928	55.241	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.19(3)	7(2)	-23(7)	0.3284	1711.633	101.896	3
3S	2.20(3)	10(1)	-22(5)	0.2638	1374.913	81.851	3
4S	2.20(3)	12(1)	-22(5)	0.2338	1218.415	72.534	3
5S	2.20(3)	14(1)	-22(4)	0.2217	1155.302	68.777	3
6S	2.21(3)	16(2)	-22(4)	0.2194	1143.243	68.059	3
7S	2.21(3)	17(2)	-22(4)	0.2225	1159.769	69.043	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.07(2)	1(1)					
1N/O	2.21(3)	2(2)	-1(3)	0.1697	884.506	59.773	5
2N/O	2.06(2)	1(2)					
2N/O	2.19(3)	2(3)	0(2)	0.1445	753.081	50.891	5
3N/O	2.08(2)	2(1)					
1N/O	2.23(3)	1(2)	1(2)	0.1424	742.049	50.146	5
4N/O	2.09(2)	5(1)					
1N/O	2.25(3)	1(3)	-1(2)	0.1423	741.754	50.126	5
3N/O	2.07(2)	3(2)					
2N/O	2.21(3)	4(4)	-1(2)	0.1455	758.183	51.236	5
5N/O	2.09(2)	7(2)					
1N/O	2.27(5)	3(5)	-1(2)	0.1562	813.907	55.002	5
4N/O	2.09(2)	7(2)					
2N/O	2.23(9)	13(14)	-1(3)	0.1580	823.709	55.664	5
3N/O	2.08(3)	6(2)					
3N/O	2.19(8)	15(10)	-1(3)	0.1585	825.902	55.812	5
6N/O	2.11(2)	10(1)					
1N/O	2.42(0.14)	16(27)	-1(3)	0.1618	843.322	56.990	5
5N/O	2.11(2)	8(2)					
2N/O	2.34(0.14)	27(34)	0(3)	0.1599	833.312	56.313	5
4N/O	2.10(2)	7(2)					
3N/O	2.26(0.17)	30(26)	0(4)	0.1614	840.999	56.833	5

Co-S(2.2) Co-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.18(2)	4(1)					
1S	2.33(3)	2(2)	-18(5)	0.2109	1098.933	74.263	5
2S	2.16(3)	5(2)					
2S	2.31(4)	6(3)	-18(4)	0.1971	1027.301	69.422	5
3S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S			No Fit	No Fit	No Fit	No Fit	5

1S							
3S	2.18(3)	8(2)					
2S	2.34(4)	8(3)	-18(4)	0.1966	1024.803	69.253	5
5S	2.21(3)	12(2)					
1S	2.39(6)	7(5)	-19(5)	0.2031	1058.369	71.522	5
4S							
2S			No Fit	No Fit	No Fit	No Fit	5
3S	2.33(5)	12(5)					
3S	2.18(3)	9(3)	-18(5)	0.2004	1044.256	70.568	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.22(2)	14(1)					
2S	2.97(3)	10(4)	-19(3)	0.1382	720.122	48.664	5
4S	2.21(3)	11(3)					
3S	2.39(7)	18(9)	-16(5)	0.1947	1014.779	68.576	5

Co-N(2.0) Co-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.05(2)	2(1)					5
1S	2.33(4)	6(3)	-6(4)	0.1974	1028.805	69.524	
1N/O	2.02(3)	1(2)					5
2S	2.28(4)	9(2)	-11(5)	0.2213	1153.471	77.949	
2N/O	2.49(4)	2(2)					
2S	2.16(2)	6(1)	-25(5)	0.2234	1164.547	78.697	5
3N/O	2.06(2)	5(1)					
1S	2.34(4)	8(4)	-5(3)	0.1757	915.555	61.871	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.12(2)	7(1)					
1S	2.69(3)	7(3)	1(2)	0.1446	753.552	50.923	5
2N/O	2.50(5)	4(3)					
3S	2.17(3)	9(1)	-25(5)	0.2152	1121.323	75.776	5

3N/O	2.07(2)	5(2)					
2S	2.35(7)	18(7)	-6(4)	0.1810	943.238	63.742	5
5N/O	2.10(2)	10(3)					
1S	1.93(7)	22(18)	1(2)	0.1526	795.558	53.762	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(2)	7(1)					
2S	2.65(6)	22(9)	1(2)	0.1477	769.687	52.013	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.50(6)	7(4)					
3S	2.17(3)	10(2)	-26(5)	0.2173	1132.475	76.530	5
6N/O	2.09(3)	10(3)					
1S	1.96(0.10)	18(18)	-1(2)	0.1558	811.970	54.871	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.12(1)	9(1)					
2S	2.67(4)	17(5)	2(2)	0.1274	664.175	44.883	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(2)	7(1)					
3S	2.62(7)	30(11)	1(2)	0.1427	743.531	50.246	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Co-N(2.0) Co-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(2)	2(1)					5
1Br	2.47(3)	10(3)	-2(5)	0.2486	1295.691	87.559	
1N/O							5
2Br			No Fit	No Fit	No Fit	No Fit	
2N/O	2.08(3)	2(2)					
2Br	2.48(4)	15(4)	-2(5)	0.2724	1419.419	95.921	5
3N/O	2.09(2)	5(1)					
1Br	2.48(3)	11(3)	-2(3)	0.1854	966.201	65.293	5

1N/O 3Br			No Fit	No Fit	No Fit	No Fit	5
1N/O 4Br	1.79(2) 2.66(5)	3(3) 25(7)	32(1)	0.3815	1988.272	134.362	5
4N/O 1Br	2.09(2) 2.47(4)	7(1) 13(4)	-2(3)	0.1574	820.441	55.443	5
2N/O 3Br	2.09(3) 2.48(5)	3(2) 20(5)	-2(5)	0.2882	1501.990	101.501	5
3N/O 2Br	2.07(4) 2.09(8)	5(2) 23(12)	-3(4)	0.2142	1116.430	75.445	5
5N/O 1Br	2.11(2) 2.44(5)	9(1) 16(6)	-1(2)	0.1453	757.205	51.170	5
1N/O 5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 2Br	2.11(2) 2.45(5)	7(2) 22(8)	-1(3)	0.1647	858.469	58.013	5
2N/O 4Br	2.09(3) 2.48(6)	3(2) 24(6)	-1(5)	0.2987	1556.816	105.206	5
3N/O 3Br	2.08(3) 2.09(9)	5(2) 31(14)	-3(4)	0.2160	1125.738	76.074	5
6N/O 1Br	2.11(2) 2.43(5)	11(2) 16(6)	-1(2)	0.1438	749.290	50.635	5
1N/O 6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O 2Br	2.11(2) 2.42(5)	9(2) 23(7)	-1(2)	0.1442	751.298	50.771	5
2N/O 5Br	2.09(3) 2.49(7)	3(2) 28(8)	-1(5)	0.3061	1595.266	107.804	5
4N/O 3Br	2.11(2) 2.43(6)	7(2) 27(9)	-1(3)	0.1665	867.718	58.638	5
3N/O 4Br	2.08(3) 2.10(0.10)	5(2) 35(15)	-3(4)	0.2172	1132.141	76.507	5

Co-N(2.0) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.13(2)	10(3)					
1Imd	2.05(4)	4(3)	-1(2)	0.1211	630.901	42.635	5
4N/O	2.12(2)	8(3)					
1Imd	1.96(8)	9(15)					
1Imd	2.06(6)	3(5)	-3(2)	0.1111	579.205	45.258	7
3N/O	2.12(2)	6(3)					
1Imd	1.94(5)	1(5)					
1Imd	2.06(4)	2(4)					
1Imd	2.21(6)	1(5)	-2(2)	0.1016	529.407	49.029	9
2N/O	2.12(3)	7(3)					
1Imd	2.16(9)	3(11)					
1Imd	2.03(5)	1(6)					
1Imd	1.91(5)	1(8)					
1Imd	1.77(0.34)	30(65)	-3(4)	0.0975	508.112	57.754	11
1N/O	2.12(3)	1(3)					
1Imd	1.93(4)	9(3)					
1Imd	2.40(7)	6(9)					
1Imd	2.04(4)	16(3)					
1Imd	2.27(4)	15(4)					
1Imd	2.15(4)	17(4)	1(2)	0.0932	485.747	71.456	13
4N/O	2.13(2)	8(2)					
1Imd	2.04(4)	4(3)	-1(2)	0.1212	631.789	42.695	5
3N/O	2.12(2)	6(3)					
1Imd	2.16(0.11)	9(14)					
1Imd	2.02(5)	3(3)	-1(2)	0.1187	618.649	48.340	7
2N/O	2.11(2)	3(3)					
1Imd	2.08(4)	3(4)					
1Imd	1.96(4)	1(4)					
1Imd	2.22(4)	2(4)	-1(2)	0.1143	595.785	55.176	9
1N/O	2.11(3)	0(3)					
1Imd	2.01(2)	13(2)					
1Imd	2.12(2)	14(2)					
1Imd	2.25(2)	10(2)					
1Imd	1.90(3)	7(3)	-2(2)	0.1190	619.985	70.470	11
0N/O							
1Imd	1.92(4)	10(5)					
1Imd	2.33(0.13)	1(26)					
1Imd	2.25(5)	14(7)					
1Imd	2.13(4)	17(6)					
1Imd	2.02(4)	16(5)	0(3)	0.1941	1011.524	114.974	11

3N/O	2.13(2)	6(3)					
1Imd	2.04(4)	3(3)	-1(3)	0.1428	744.367	50.302	5
2N/O	2.12(3)	4(3)					
1Imd	2.18(6)	4(6)					
1Imd	2.03(4)	1(2)	0(3)	0.1448	754.740	58.974	7
1N/O	2.10(3)	0(3)					
1Imd	1.98(4)	3(4)					
1Imd	2.23(4)	4(3)					
1Imd	2.10(4)	5(4)	-1(3)	0.1532	798.402	73.941	9
0N/O							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O	2.12(3)	4(3)					
1Imd	2.05(4)	2(3)	-1(3)	0.2002	1043.259	70.501	5
1N/O	2.10(4)	0(4)					
1Imd	2.03(4)	0(4)					
1Imd	2.18(5)	1(4)	0(3)	0.2089	1088.597	85.061	7
0N/O							
1Imd	2.00(4)	4(4)					
1Imd	2.23(4)	5(5)					
1Imd	2.11(4)	7(4)	0(3)	0.2788	1452.994	113.534	7

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.15(2)	9(2)					
1S	2.68(2)	7(2)					
1Imd	2.06(2)	2(2)	1(2)	0.0842	438.837	34.290	7
3N/O	2.13(2)	6(2)					
1S	2.69(2)	6(2)					
1Imd	2.25(4)	4(4)					
1Imd	2.07(2)	1(2)	2(1)	0.0699	364.336	33.742	9
2N/O	2.06(3)	1(2)					
1S	2.34(4)	5(3)					
1Imd	1.90(6)	4(11)					
1Imd	1.82(0.32)	32(126)					
1Imd	2.03(7)	4(13)	-8(5)	0.1082	520.508	59.163	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

4N/O	2.15(2)	9(2)					
1S	2.69(2)	7(2)					
1Imd	2.06(2)	2(2)	1(2)	0.0805	419.506	32.779	7
3N/O	2.08(3)	4(2)					
1S	2.35(4)	8(4)					
1Imd	2.02(5)	2(5)					
1Imd	1.88(4)	4(5)	-7(3)	0.1098	572.225	52.994	9
2N/O	2.06(3)	1(2)					
1S	2.34(4)	5(3)					
1Imd	1.81(0.31)	32(0.123)					
1Imd	2.03(7)	4(13)					
1Imd	1.90(6)	4(11)	-8(5)	0.1115	581.127	66.053	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.15(2)	9(2)					
1S	2.69(2)	7(2)					
1Imd	2.06(2)	2(2)	1(1)	0.0774	403.467	31.526	7
3N/O	2.08(3)	4(2)					
1S	2.35(4)	9(5)					
1Imd	2.02(5)	2(5)					
1Imd	1.88(4)	4(6)	-7(3)	0.1113	580.214	53.734	9
2N/O	2.06(3)	1(2)					
1S	2.34(4)	5(3)					
1Imd	2.02(8)	4(14)					
1Imd	1.80(0.32)	32(120)					
1Imd	1.90(7)	4(12)	-9(5)	0.1140	594.324	67.553	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.14(2)	9(2)					
1S	2.69(2)	7(2)					
1Imd	2.07(2)	3(2)	1(1)	0.0754	393.111	30.717	7
3N/O	2.13(2)	7(2)					
1S	2.69(2)	7(2)					
1Imd	2.25(4)	4(4)					
1Imd	2.07(2)	1(2)	2(1)	0.0615	320.558	29.687	9
2N/O	2.12(2)	4(3)					
1S	2.69(2)	5(2)					
1Imd	2.15(3)	5(3)					
1Imd	2.29(3)	3(3)					
1Imd	2.02(3)	3(3)	2(2)	0.0625	325.838	37.036	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.14(2)	9(2)					
1S	2.69(2)	7(2)					
1Imd	2.06(2)	3(2)	1(1)	0.0738	384.662	30.057	7
3N/O	2.13(2)	7(2)					
1S	2.69(2)	7(2)					
1Imd	2.24(4)	4(4)					
1Imd	2.06(2)	1(2)	2(1)	0.0599	312.371	28.929	9
2N/O	2.12(2)	4(3)					
1S	2.69(2)	6(2)					
1Imd	2.02(3)	3(3)					
1Imd	2.15(3)	5(3)					
1Imd	2.29(3)	3(3)	2(1)	0.0614	320.088	36.382	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.14(3)	10(3)					
1Br	2.44(4)	14(5)					
1Imd	2.06(3)	2(2)	0(2)	0.1031	537.268	41.981	7
3N/O	2.13(3)	8(3)					
1Br	2.45(3)	13(4)					
1Imd	2.27(5)	5(6)					
1Imd	2.07(3)	1(2)	1(2)	0.0953	496.563	45.987	9
2N/O	2.13(3)	5(4)					
1Br	2.45(3)	10(4)					
1Imd	2.02(4)	2(4)					
1Imd	2.16(5)	4(4)					
1Imd	2.31(5)	3(4)	2(2)	0.0894	465.801	52.945	11

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.15(3)	10(3)					
1Br	2.45(3)	14(5)					
1Imd	2.06(3)	2(2)	0(2)	0.1009	525.774	41.083	7
3N/O	2.13(3)	7(3)					
1Br	2.45(3)	13(4)					
1Imd	2.27(5)	4(6)					
1Imd	2.07(3)	1(2)	1(2)	0.0926	482.404	44.676	9
2N/O	2.13(3)	5(4)					
1Br	2.45(3)	10(4)					
1Imd	2.31(5)	3(4)					
1Imd	2.03(4)	2(3)					
1Imd	2.16(5)	4(4)	2(2)	0.0864	450.479	51.203	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.14(3)	10(3)					
1Br	2.45(3)	14(4)					
1Imd	2.06(3)	2(2)	0(2)	0.0989	515.411	40.273	7
3N/O	2.13(3)	7(3)					
1Br	2.46(3)	13(4)					
1Imd	2.27(5)	4(5)					
1Imd	2.07(3)	2(2)	1(2)	0.0902	470.353	43.560	9
2N/O	2.12(3)	5(4)					
1Br	2.45(3)	5(4)					
1Imd	2.03(4)	2(3)					
1Imd	2.16(5)	4(4)					
1Imd	2.31(5)	3(4)	2(2)	0.0840	437.631	49.743	11

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.14(3)	10(3)					
1Br	2.45(3)	14(4)					
1Imd	2.06(3)	2(2)	0(2)	0.0973	506.872	39.606	7
3N/O	2.13(3)	7(3)					
1Br	2.46(3)	13(4)					
1Imd	2.07(3)	2(2)					
1Imd	2.27(5)	4(5)	1(2)	0.0884	460.928	42.687	9
2N/O	2.12(3)	5(4)					
1Br	2.46(3)	10(3)					
1Imd	2.16(5)	4(4)					
1Imd	2.03(4)	2(3)					
1Imd	2.31(4)	3(4)	2(2)	0.0821	427.924	48.640	11

Co-N(2.0) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(3)	7(4)					
2Br	2.44(5)	22(8)					
1Imd	2.05(3)	2(3)	0(3)	0.1338	697.274	54.484	7
2N/O	2.13(3)	5(4)					
2Br	2.44(4)	19(6)					
1Imd	2.24(5)	3(5)					
1Imd	2.06(4)	1(2)	2(2)	0.1283	668.746	61.933	9
1N/O	2.13(5)	2(5)					
2Br	2.44(4)	16(5)					
1Imd	2.02(4)	4(3)	2(2)	0.1321	688.356	78.241	11

1Imd	2.15(4)	6(4)					
1Imd	2.29(5)	5(4)					

Co-N(2.0) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(3)	7(4)					
2Br	2.44(5)	22(7)					
1Imd	2.05(3)	2(3)	0(2)	0.1312	683.717	53.424	7
2N/O	2.13(3)	5(4)					
2Br	2.45(4)	19(6)					
1Imd	2.24(5)	3(4)					
1Imd	2.06(4)	1(2)	2(2)	0.1250	651.252	60.313	9
1N/O	2.12(5)	2(5)					
2Br	2.44(4)	16(5)					
1Imd	2.29(4)	5(3)					
1Imd	2.15(4)	6(3)					
1Imd	2.02(4)	4(3)	2(2)	0.1284	669.154	76.059	11

Co-N(2.0) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(3)	7(4)					
2Br	2.44(5)	22(7)					
1Imd	2.05(3)	2(3)	0(2)	0.1287	670.793	52.415	7
2N/O							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.12(5)	2(5)					
2Br	2.44(4)	16(5)					
1Imd	2.29(4)	5(3)					
1Imd	2.15(4)	6(3)					
1Imd	2.02(4)	4(3)	2(2)	0.1253	652.791	74.199	11

Co-N(2.0) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(3)	7(4)					
2Br	2.45(4)	21(7)					
1Imd	2.05(3)	2(3)	0(2)	0.1266	659.888	51.562	7
2N/O	2.13(3)	5(4)					
2Br	2.45(4)	19(5)					
1Imd	2.24(5)	3(4)					
1Imd	2.06(3)	1(2)	1(2)	0.1197	624.019	57.791	9
1N/O	2.12(4)	2(5)					
2Br	2.44(4)	16(5)	2(2)	0.1230	641.228	72.885	11

1Imd	2.29(4)	5(3)					
1Imd	2.02(4)	4(3)					
1Imd	2.15(4)	6(3)					

Co-N(2.0) Co-Br(2.3) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(3)	1(3)					
1Br	2.23(5)	6(3)					
1Br	2.44(4)	6(2)					
1Imd	2.04(4)	4(3)	-1(2)	0.0643	334.993	31.024	9
2N/O							
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
1N/O	2.09(3)	9(2)					
1Br	2.20(4)	1(3)					
1Br	2.40(3)	1(2)					
1Imd	1.99(2)	7(1)					
1Imd	2.13(2)	7(2)					
1Imd	2.26(4)	0(6)	0(2)	0.0412	214.769	31.594	13

Co-N(2.0) Co-Br(2.3) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(3)	1(3)					
1Br	2.23(5)	6(3)					
1Br	2.44(4)	7(2)					
1Imd	2.04(4)	4(3)	-1(2)	0.0623	324.748	30.075	9
2N/O	2.11(2)	5(2)					
1Br	2.22(3)	0(2)					
1Br	2.41(3)	3(2)					
1Imd	2.14(2)	3(1)					
1Imd	1.98(2)	4(1)	-1(1)	0.0319	166.492	18.924	11
1N/O	2.09(3)	9(2)					
1Br	2.20(4)	1(3)					
1Br	2.40(3)	2(2)					
1Imd	1.99(2)	7(1)					
1Imd	2.13(2)	7(2)					
1Imd	2.26(4)	0(6)	0(2)	0.0403	210.282	30.934	13

Co-N(2.0) Co-Br(2.3) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	1(2)					
1Br	2.23(5)	6(3)					
1Br	2.44(4)	7(2)	-1(2)	0.0607	316.420	29.304	9

1Imd	2.04(4)	4(3)					
2N/O	2.11(2)	5(2)					
1Br	2.22(3)	0(2)					
1Br	2.41(2)	3(2)					
1Imd	2.14(2)	3(1)					
1Imd	1.98(2)	4(1)	-2(1)	0.0307	160.182	18.207	11
1N/O	2.09(3)	9(2)					
1Br	2.20(4)	0(3)					
1Br	2.40(3)	2(2)					
1Imd	1.99(2)	7(1)					
1Imd	2.13(2)	7(2)					
1Imd	2.26(4)	1(6)	0(2)	0.0397	206.685	30.404	13

Co-N(2.0) Co-Br(2.4) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(3)	2(3)					
1Br	2.44(4)	6(2)					
1Br	2.24(5)	6(3)					
1Imd	2.03(4)	4(3)	-1(2)	0.0644	335.424	31.064	9
2N/O	2.11(2)	5(2)					
1Br	2.22(3)	0(2)					
1Br	2.41(2)	2(2)					
1Imd	2.14(2)	2(1)					
1Imd	1.98(2)	4(1)	-2(1)	0.0314	163.550	18.590	11
1N/O	2.10(3)	9(2)					
1Br	2.21(3)	1(3)					
1Br	2.41(3)	1(2)					
1Imd	2.13(2)	7(2)					
1Imd	2.26(4)	1(7)					
1Imd	1.99(2)	7(1)	0(2)	0.0392	204.293	30.053	13

Co-N(2.0) Co-Br(2.4) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.13(3)	7(3)					
1Br	2.53(6)	16(9)					
1Br	2.80(3)	9(3)					
1Imd	2.05(3)	1(2)	-1(2)	0.0842	438.661	40.625	9
2N/O	2.12(2)	5(2)					
1Br	2.41(3)	2(2)					
1Br	2.23(3)	0(2)					
1Imd	1.98(2)	4(1)					
1Imd	2.14(2)	2(2)	-2(2)	0.0341	177.855	20.216	11
1N/O	2.10(3)	9(2)					
1Br	2.41(3)	0(2)	0(2)	0.0390	29.920	203.393	13

1Br	2.21(3)	1(3)					
1Imd	1.99(2)	7(1)					
1Imd	2.14(2)	6(2)					
1Imd	2.26(4)	1(7)					

Co-N(2.0) Co-Br(2.5) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(3)	2(3)					
1Br	2.44(4)	6(2)					
1Br	2.24(5)	6(3)					
1Imd	2.03(4)	4(3)	-1(2)	0.0625	325.913	30.183	9
2N/O	2.14(3)	5(5)					
1Br	2.56(0.11)	19(16)					
1Br	2.81(4)	7(3)					
1Imd	2.14(7)	4(10)					
1Imd	2.03(4)	0(3)	0(2)	0.0786	409.804	46.580	11
1N/O	2.09(5)	2(5)					
1Br	2.16(5)	9(7)					
1Br	2.78(4)	7(3)					
1Imd	1.98(0.36)	1(13)					
1Imd	2.15(0.80)	1(76)					
1Imd	2.06(0.49)	0(123)	-3(3)	0.0763	397.722	58.507	13

Co-N(2.0) Co-S(2.2) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(1)	5(2)					
1S	2.51(3)	4(2)					
1Br	2.46(2)	0(2)					
1Imd	2.06(3)	3(3)	-1(1)	0.0398	207.313	19.199	9
2N/O	2.09(1)	2(1)					
1S	2.49(3)	4(2)					
1Br	2.45(3)	1(2)					
1Imd	2.16(6)	8(9)					
1Imd	2.02(4)	2(3)	-1(1)	0.0310	161.344	18.339	11
1N/O	2.09(1)	3(1)					
1S	2.47(4)	4(4)					
1Br	2.43(3)	0(3)					
1Imd	2.25(8)	6(16)					
1Imd	2.12(3)	1(6)					
1Imd	1.98(2)	2(2)	-1(2)	0.0287	149.471	21.988	13

Co-N(2.0) Co-S(2.2) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(1)	5(2)					
1S	2.51(3)	4(2)	-1(1)	0.0376	195.818	18.135	9

1Br	2.47(2)	0(2)					
1Imd	2.06(3)	3(3)					
2N/O	2.10(1)	2(1)					
1S	2.49(3)	3(2)					
1Br	2.45(3)	0(2)					
1Imd	2.16(4)	6(6)					
1Imd	2.01(3)	2(2)	-1(1)	0.0296	154.070	17.512	11
1N/O	2.09(1)	3(1)					
1S	2.47(4)	3(4)					
1Br	2.43(3)	1(3)					
1Imd	1.98(2)	2(2)					
1Imd	2.25(7)	6(15)					
1Imd	2.12(3)	2(5)	-1(2)	0.0276	144.066	21.193	13

Co-N(2.0) Co-S(2.2) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.17(5)	12(7)					
1S	1.84(6)	22(10)					
1Br	2.46(3)	13(4)					
1Imd	2.08(3)	2(2)	2(3)	0.0896	466.925	43.242	9
2N/O	2.10(1)	2(1)					
1S	2.49(3)	3(2)					
1Br	2.45(3)	1(2)					
1Imd	2.01(3)	2(2)					
1Imd	2.15(4)	5(5)	-1(1)	0.0287	149.777	17.024	11
1N/O	2.09(1)	3(1)					
1S	2.46(4)	2(3)					
1Br	2.43(3)	1(3)					
1Imd	1.98(2)	2(2)					
1Imd	2.12(3)	2(4)					
1Imd	2.25(7)	6(15)	-1(2)	0.0267	139.053	20.455	13

Co-N(2.0) Co-S(2.2) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(1)	5(2)					
1S	2.51(3)	2(3)					
1Br	2.47(3)	1(2)					
1Imd	2.06(3)	4(3)	-1(1)	0.0372	193.694	17.938	9
2N/O	2.10(1)	2(1)					
1S	2.48(3)	2(2)					
1Br	2.45(3)	1(2)					
1Imd	2.15(4)	4(4)					
1Imd	2.00(3)	1(2)	-1(1)	0.0278	145.057	16.488	11
1N/O	2.09(1)	3(1)	-1(2)	0.0256	133.208	19.596	13

1S	2.46(3)	2(3)					
1Br	2.43(3)	1(2)					
1Imd	2.12(3)	2(4)					
1Imd	1.98(2)	2(2)					
1Imd	2.25(7)	7(16)					

Co-N(2.0) Co-S(2.3) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	4(1)					
1S	2.51(3)	4(3)					
1Br	2.46(3)	0(2)					
1Imd	2.05(4)	4(3)	-1(1)	0.0407	212.144	19.647	9
2N/O	2.09(1)	2(1)					
1S	2.50(3)	5(2)					
1Br	2.45(2)	1(2)					
1Imd	2.14(8)	12(17)					
1Imd	2.03(5)	3(3)	-1(1)	0.0301	157.109	17.858	11
1N/O	2.09(1)	3(1)					
1S	2.48(4)	4(4)					
1Br	2.44(3)	1(3)					
1Imd	2.26(6)	5(12)					
1Imd	1.98(2)	2(2)					
1Imd	2.12(3)	2(5)	-1(2)	0.0272	141.888	20.873	13

Co-N(2.0) Co-S(2.3) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(1)	5(1)					
1S	2.52(3)	4(2)					
1Br	2.47(2)	0(2)					
1Imd	2.06(3)	3(3)	-1(1)	0.0368	191.592	17.744	9
2N/O	2.09(1)	2(1)					
1S	2.50(3)	4(2)					
1Br	2.46(2)	1(2)					
1Imd	2.15(6)	9(11)					
1Imd	2.02(4)	3(3)	-1(1)	0.0284	147.760	16.795	11
1N/O	2.09(1)	3(1)					
1S	2.48(4)	3(4)					
1Br	2.44(3)	0(3)					
1Imd	2.12(3)	2(4)					
1Imd	1.98(2)	2(2)					
1Imd	2.26(6)	5(12)	-1(2)	0.0261	136.061	20.015	13

Co-N(2.0) Co-S(2.3) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(1)	5(2)	-1(1)	0.0354	184.333	17.071	9

1S	2.52(3)	4(2)					
1Br	2.47(2)	0(2)					
1Imd	2.06(3)	3(3)					
2N/O	2.09(1)	2(1)					
1S	2.50(3)	3(3)					
1Br	2.45(3)	0(2)					
1Imd	2.01(4)	2(3)					
1Imd	2.15(4)	6(7)	-1(1)	0.0275	143.364	16.295	11
1N/O	2.09(1)	3(1)					
1S	2.47(4)	3(4)					
1Br	2.44(3)	1(3)					
1Imd	2.26(6)	6(13)					
1Imd	1.98(2)	2(2)					
1Imd	2.12(3)	2(4)	-1(2)	0.0251	131.043	19.277	13

Co-N(2.0) Co-S(2.3) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(1)	5(2)					
1S	2.52(3)	3(3)					
1Br	2.47(2)	0(2)					
1Imd	2.06(3)	4(3)	-1(1)	0.0350	182.429	16.895	9
2N/O	2.10(1)	2(1)					
1S	2.49(3)	3(3)					
1Br	2.45(3)	1(2)					
1Imd	2.01(3)	2(2)					
1Imd	2.15(4)	5(5)	-1(1)	0.0266	138.728	15.768	11
1N/O	2.09(1)	3(1)					
1S	2.47(3)	2(3)					
1Br	2.43(3)	1(3)					
1Imd	1.98(2)	2(2)					
1Imd	2.25(7)	6(14)					
1Imd	2.12(3)	2(4)	-1(1)	0.0240	125.046	18.395	13

Co-N(2.0) Co-S(2.4) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.09(1)	1(1)					
1S	2.51(2)	5(2)					
1Br	2.46(2)	2(2)					
1Imd	2.04(5)	4(5)					
1Imd	2.09(0.14)	16(20)	-2(1)	0.0287	149.829	17.030	11

1N/O	2.08(2)	2(3)					
1S	2.47(4)	9(3)					
1Br	2.42(4)	5(3)					
1Imd	2.17(5)	2(5)					
1Imd	2.02(4)	5(5)					
1Imd	1.93(6)	5(8)	-3(2)	0.0259	134.791	19.828	13

Co-N(2.0) Co-S(2.4) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.09(1)	2(1)					
1S	2.51(2)	5(2)					
1Br	2.46(2)	1(2)					
1Imd	2.12(0.10)	14(19)					
1Imd	2.04(6)	4(4)	-1(1)	0.0267	139.035	15.803	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.4) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.09(1)	2(1)					
1S	2.51(3)	4(2)					
1Br	2.46(2)	1(2)					
1Imd	2.14(6)	9(13)					
1Imd	2.02(6)	3(3)	-1(1)	0.0260	135.506	15.402	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.4) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

3N/O							
1S							
1Br							
1Imd							9
2N/O	2.09(1)	2(1)					
1S	2.50(3)	4(3)					
1Br	2.46(2)	0(2)					
1Imd	2.01(4)	3(3)					
1Imd	2.14(4)	7(8)	-1(1)	0.0253	132.002	15.004	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.5) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.08(1)	1(1)					
1S	2.51(2)	6(2)					
1Br	2.45(2)	3(2)					
1Imd	2.06(6)	3(4)					
1Imd	1.98(7)	10(13)	-3(1)	0.0234	121.719	13.835	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.5) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.09(1)	1(1)					
1S	2.51(1)	6(2)					
1Br	2.46(1)	2(2)					
1Imd	2.06(0.11)	16(14)					
1Imd	2.05(4)	4(4)	-2(1)	0.0215	112.160	12.749	11

1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.5) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.09(1)	2(1)					
1S	2.51(2)	5(2)					
1Br	2.46(1)	2(2)					
1Imd	2.04(4)	4(4)					
1Imd	2.10(0.10)	15(15)	-2(1)	0.0212	110.281	12.535	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.5) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.09(1)	2(1)					
1S	2.51(2)	5(2)					
1Br	2.46(2)	1(2)					
1Imd	2.12(7)	11(15)					
1Imd	2.03(6)	4(3)	-2(1)	0.0211	109.915	12.493	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.6) Co-Br(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1Br							
1Imd							9
2N/O	2.08(2)	4(1)					
1S	2.62(2)	4(2)					
1Br	2.17(2)	3(2)					
1Imd	2.12(2)	2(1)					
1Imd	1.97(2)	3(1)	-2(1)	0.0274	142.648	16.214	11
1N/O							
1S							
1Br							
1Imd							
1Imd							
1Imd							13

Co-N(2.0) Co-S(2.6) Co-Br(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	4(1)					
1S	2.52(2)	4(2)					
1Br	2.47(2)	0(2)					
1Imd	2.04(4)	6(4)	-2(1)	0.0363	189.311	17.532	9
2N/O	2.09(1)	1(1)					
1S	2.51(2)	6(2)					
1Br	2.46(1)	2(1)					
1Imd	2.00(0.10)	11(16)					
1Imd	2.06(9)	4(5)	-3(1)	0.0200	104.001	11.821	11
1N/O	2.08(1)	3(1)					
1S	2.50(2)	8(2)					
1Br	2.45(2)	4(2)					
1Imd	1.97(7)	2(12)					
1Imd	2.07(8)	1(11)					
1Imd	2.20(6)	3(12)	-2(2)	0.0177	85.065	12.514	13

Co-N(2.0) Co-S(2.6) Co-Br(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	4(1)					
1S	2.52(2)	4(2)					
1Br	2.47(2)	0(2)					
1Imd	2.05(3)	5(3)	-2(1)	0.0327	170.371	15.778	9
2N/O	2.09(1)	1(1)					
1S	2.51(2)	5(2)					
1Br	2.46(1)	2(2)					
1Imd	2.07(0.11)	14(13)	-2(1)	0.0194	101.094	11.491	11

1Imd	2.04(5)	5(5)					
1N/O	2.08(1)	3(1)					
1S	2.50(3)	7(2)					
1Br	2.45(2)	3(2)					
1Imd	2.19(0.11)	3(18)					
1Imd	2.04(0.32)	1(13)					
1Imd	2.01(0.43)	5(46)	-2(2)	0.0190	99.065	14.573	13

Co-N(2.0) Co-S(2.6) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	5(1)					
1S	2.52(2)	4(2)					
1Br	2.47(2)	1(2)					
1Imd	2.05(3)	4(3)	-2(1)	0.0306	159.429	14.765	9
2N/O	2.09(1)	2(1)					
1S	2.51(2)	5(2)					
1Br	2.46(2)	1(2)					
1Imd 0°	2.03(6)	4(4)					
1Imd 0°	2.09(9)	12(15)	-2(1)	0.0192	100.191	11.388	11
2N/O	2.09(1)	2(1)					
1S	2.51(2)	5(2)					
1Br	2.46(1)	1(2)					
1Imd 0°	2.04(4)	4(4)					
1Imd 5°	2.06(0.11)	13(13)	-2(1)	0.0196	102.101	11.605	11
2N/O	2.09(1)	2(1)					
1S	2.51(2)	5(2)					
1Br	2.46(2)	2(2)					
1Imd 0°	2.04(3)	3(3)					
1Imd 10°	2.06(0.16)	16(18)	-2(1)	0.0215	111.945	12.724	11
2N/O	2.08(2)	2(2)					
1S	2.50(2)	4(2)					
1Br	2.45(2)	1(2)					
1Imd 5°	2.03(3)	4(3)					
1Imd 10°	2.16(6)	7(7)	-2(1)	0.0262	136.435	15.508	11
1N/O	2.09(1)	3(1)					
1S	2.49(3)	5(2)					
1Br	2.45(3)	2(2)					
1Imd	2.09(0.40)	17(33)					
1Imd	2.00(4)	0(4)					
1Imd	2.15(0.12)	4(9)	-2(2)	0.0193	100.834	14.833	13

Co-N(2.2) Co-S(2.6) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	2(1)	-2(1)	0.0211	109.849	12.486	11

1S	2.51(2)	5(2)					
1Br	2.46(2)	1(2)					
1Imd 0°	2.08(0.11)	17(13)					
1Imd 0°	2.04(3)	3(3)					

Co-N(2.0) Co-N(2.2) Co-S(2.6) Co-Br(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.10(3)	3(2)					
1N/O	2.02(6)	7(12)					
1S	2.51(2)	7(2)					
1Br	2.46(2)	3(2)					
1Imd	2.02(3)	0(3)					
1Imd	2.17(6)	6(7)	-2(1)	0.0159	82.942	12.201	13
1N/O	2.10(1)	2(1)					
1N/O	2.06(9)	15(17)					
1S	2.50(2)	5(3)					
1Br	2.46(2)	1(2)					
1Imd	2.13(3)	3(5)					
1Imd	2.00(3)	1(2)	-2(1)	0.0157	82.077	12.074	13
1N/O	2.04(2)	5(2)					
1N/O	2.15(1)	6(2)					
1S	2.53(2)	8(2)					
1Br	2.49(2)	4(2)					
1Imd	2.06(2)	1(2)					
1Imd	1.93(3)	0(3)	-3(1)	0.0163	84.780	12.472	13
1N/O	2.03(2)	5(2)					
1N/O	2.15(2)	6(2)					
1S	2.53(3)	8(3)					
1Br	2.49(3)	4(3)					
1Imd	2.07(3)	2(3)					
1Imd	1.92(3)	0(3)	-3(1)	0.0244	127.285	18.724	13

Table G.5. Additional Fits for Zn(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.14(3)	2(4)	13(1)	0.5029	11915.663	1753.109	3
3N/O	2.11(5)	4(4)	9(6)	0.4487	10632.943	1564.387	3
4N/O	2.10(5)	6(4)	7(6)	0.4332	10265.242	1510.289	3
5N/O	2.08(5)	8(4)	4(6)	0.4400	10425.709	1533.897	3
6N/O	2.07(5)	10(4)	2(6)	0.4593	10884.157	1601.347	3
7N/O	2.06(6)	12(5)	1(6)	0.4852	11497.642	1691.607	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.26(3)	5(2)	0(6)	0.2615	6196.113	911.612	3
3S	2.24(3)	8(2)	neg4(6)	0.2306	5465.036	804.051	3
4S	2.23(3)	10(2)	neg7(5)	0.2331	5523.718	812.685	3
5S	2.22(4)	12(2)	neg9(6)	0.2520	5970.846	878.469	3
6S	2.21(4)	14(2)	neg11(6)	0.2786	6602.008	971.330	3
7S	2.20(4)	15(3)	neg13(6)	0.3084	7306.607	1074.995	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.04(3)	2(3)					
1N/O	2.17(3)	6(2)	7(5)	0.2378	5634.203	1174.557	5
2N/O	2.00(3)	2(3)					
2N/O	2.15(3)	3(2)	4(5)	0.2738	6488.158	1352.580	5
3N/O	2.04(3)	1(3)					
1N/O	2.17(3)	6(2)	5(5)	0.2502	5927.608	1235.723	5
4N/O	2.03(4)	3(3)					
1N/O	2.17(3)	5(2)	3(5)	0.2871	6802.359	1418.081	5
3N/O	2.01(4)	1(3)					
2N/O	2.15(3)	3(3)	3(5)	0.3153	7472.297	1557.743	5
5N/O	2.03(4)	5(4)					
1N/O	2.17(3)	4(3)	1(5)	0.3348	7932.534	1653.688	5
4N/O	2.00(4)	3(4)					
2N/O	2.15(4)	2(3)	1(5)	0.3653	8657.073	1804.732	5
3N/O	1.98(4)	2(4)					
3N/O	2.13(4)	0(3)	1(5)	0.3909	9262.333	1930.910	5
6N/O	2.02(5)	8(4)					
1N/O	2.16(4)	3(3)	0(6)	0.3852	9126.870	1902.670	5
5N/O	2.00(5)	6(5)					
2N/O	2.15(4)	1(4)	neg1(6)	0.4161	9859.027	2055.302	5
4N/O	1.98(6)	5(5)					
3N/O	2.13(5)	1(4)	neg1(6)	0.4419	10470.892	2182.857	5

Zn-S(2.2) Zn-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.14(2)	3(2)					
1S	2.27(2)	2(1)	neg11(4)	0.0767	1816.652	378.716	5

2S	2.11(3)	3(2)					
2S	2.26(2)	1(1)	neg13(4)	0.1038	2459.097	512.646	5
3S	2.14(3)	6(2)					
1S	2.27(2)	1(1)	neg13(4)	0.0944	2237.981	466.550	5
4S	2.22(3)	5(2)					
1S	2.06(3)	1(2)	neg12(5)	0.1473	3489.649	727.484	5
3S	2.11(3)	6(2)					
2S	2.26(3)	2(2)	neg14(5)	0.1408	3337.155	695.693	5
5S	2.23(6)	12(4)					
1S	1.82(0.12)	20(25)	neg5(9)	0.2294	5435.045	1133.039	5
4S	2.23(3)	5(2)					
2S	2.07(4)	4(3)	neg14(5)	0.1870	4431.007	923.728	5
3S	2.09(4)	7(3)					
3S	2.24(3)	4(2)	neg15(6)	0.1946	4610.512	961.149	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.24(6)	12(4)					
2S	1.84(9)	27(21)	neg3(10)	0.2166	5131.666	1069.793	5
4S	2.23(4)	6(3)					
3S	2.08(5)	8(4)	neg16(6)	0.2285	5414.539	1128.764	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	1(2)					5
1S	2.28(2)	1(1)	0(4)	0.0858	2033.578	423.938	
1N/O	1.96(2)	2(2)					5
2S	2.26(2)	3(1)	neg4(4)	0.0973	2305.216	480.566	
2N/O	1.97(3)	2(3)					
2S	2.26(3)	3(2)	neg4(4)	0.1356	3212.741	669.757	5
3N/O	2.01(3)	4(2)					
1S	2.28(2)	0(1)	neg1(4)	0.1135	2690.624	560.912	5
1N/O	1.94(3)	1(3)					
3S	2.24(3)	6(2)	neg6(5)	0.1492	3536.454	737.241	5
1N/O	2.18(2)	5(1)					
4S	2.19(2)	6(1)	neg10(4)	0.0832	1971.679	411.034	5

4N/O	2.01(4)	7(3)					
1S	2.28(3)	0(2)	neg1(5)	0.1535	3637.828	758.374	5
2N/O	2.13(0.16)	17(89)					
3S	2.25(4)	8(6)	0(15)	0.2048	4852.030	1011.498	5
3N/O	2.13(0.19)	16(35)					
2S	2.27(4)	6(5)	4(15)	0.1867	4424.622	922.397	5
5N/O	2.02(7)	11(5)					
1S	2.28(3)	1(2)	neg1(6)	0.1930	4573.818	953.500	5
1N/O	2.17(2)	4(2)					
5S	2.19(2)	8(2)	neg11(4)	0.1064	2522.217	525.804	5
4N/O	2.19(0.13)	21(39)					
2S	2.28(4)	5(2)	7(14)	0.1793	4247.767	885.528	5
2N/O	2.18(2)	3(1)					
4S	2.19(2)	5(1)	neg9(4)	0.0709	1679.671	350.159	5
3N/O	2.19(0.13)	17(83)					
3S	2.27(4)	8(4)	3(18)	0.1910	4526.854	943.709	5
6N/O	2.04(0.12)	16(7)					
1S	2.27(3)	2(3)	0(9)	0.2244	5318.172	1108.674	5
1N/O	2.16(3)	4(2)					
6S	2.18(3)	10(2)	neg13(5)	0.1423	3371.410	702.835	5
5N/O	2.22(0.10)	26(28)					
2S	2.29(3)	5(2)	8(10)	0.1722	4080.214	850.598	5
2N/O	2.18(2)	3(1)					
5S	2.18(2)	7(1)	neg11(4)	0.0846	2005.575	418.100	5
4N/O	2.23(9)	18(36)					
3S	2.28(3)	7(2)	6(10)	0.1739	4120.757	859.050	5
3N/O	2.19(2)	3(1)					
4S	2.19(2)	4(1)	neg7(5)	0.0692	1640.917	342.080	5

Zn-N(2.0) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.01(4)	2(2)					5
1Br	2.38(3)	3(1)	neg4(6)	0.0860	2037.976	424.855	
1N/O	1.95(3)	1(2)	neg14(7)	0.0935	2216.072	461.982	5

2Br	2.35(3)	7(1)					
2N/O	1.97(3)	3(2)					
2Br	2.37(2)	7(1)	neg10(5)	0.0453	1073.437	223.778	5
3N/O	2.02(3)	5(2)					
1Br	2.39(2)	4(1)	neg3(4)	0.0490	1161.892	242.218	5
1N/O	1.93(3)	1(2)					
3Br	2.34(2)	9(1)	neg16(5)	0.0649	1537.705	320.564	5
1N/O	1.92(2)	0(2)					
4Br	2.34(2)	11(1)	neg18(5)	0.0548	1298.855	270.771	5
4N/O	2.02(2)	7(2)					
1Br	2.39(1)	4(1)	neg3(3)	0.0399	944.404	196.879	5
2N/O	1.95(2)	3(1)					
3Br	2.36(2)	9(1)	neg12(4)	0.0353	836.332	174.349	5
3N/O	1.99(2)	6(1)					
2Br	2.38(1)	7(1)	neg7(3)	0.0246	581.972	121.323	5
5N/O	2.02(3)	9(2)					
1Br	2.39(1)	4(1)	neg3(3)	0.0470	1112.639	231.951	5
1N/O	2.40(3)	4(1)					
5Br	2.25(3)	13(2)	neg32(7)	0.0756	1792.491	373.679	5
4N/O	2.00(2)	8(1)					
2Br	2.39(1)	7(1)	neg6(3)	0.0207	491.292	102.419	5
2N/O	1.94(2)	4(2)					
4Br	2.36(2)	11(1)	neg14(4)	0.0380	900.056	187.634	5
3N/O	1.97(2)	6(1)					
3Br	2.37(1)	9(1)	neg9(3)	0.0251	595.359	124.114	5
6N/O	2.02(3)	11(2)					
1Br	2.39(2)	4(1)	neg4(4)	0.0625	1481.476	308.842	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.01(3)	10(2)					
2Br	2.39(1)	7(1)	neg5(3)	0.0273	646.464	134.768	5
2N/O	1.93(3)	4(2)					
5Br	2.35(2)	12(1)	neg16(4)	0.4650	1102.328	229.801	5

4N/O	1.99(3)	9(2)					
3Br	2.38(1)	10(1)	neg7(3)	0.0248	586.732	122.315	5
3N/O	1.96(3)	7(2)					
4Br	2.37(2)	11(1)	neg11(4)	0.0346	820.006	170.946	5

Table G.6. Additional Fits for Zn(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(2)	2(3)	12(0)	0.5408	13901.569	827.580	3
3N/O	2.11(2)	4(3)	9(0)	0.4878	12537.136	746.354	3
4N/O	2.10(3)	7(3)	7(4)	0.4719	12130.613	722.153	3
5N/O	2.08(3)	8(3)	4(4)	0.4776	12276.803	730.856	3
6N/O	2.07(4)	10(3)	2(4)	0.4956	12739.131	758.379	3
7N/O	2.06(4)	12(3)	1(4)	0.5199	13364.269	795.594	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.26(2)	5(1)	0(5)	0.3171	8150.660	485.220	3
3S	2.24(2)	8(1)	-4(4)	0.2864	7362.694	438.312	3
4S	2.23(2)	10(1)	-7(4)	0.2876	7393.045	440.118	3
5S	2.22(3)	12(2)	-9(4)	0.3046	7829.518	466.102	3
6S	2.21(3)	14(2)	-11(4)	0.3291	8460.015	503.637	3
7S	2.20(3)	15(2)	-13(5)	0.3567	9169.112	545.850	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.04(2)	2(2)					
1N/O	2.18(2)	6(1)	7(3)	0.3149	8093.365	546.928	5
2N/O	2.00(2)	2(2)					
2N/O	2.15(2)	3(2)	4(3)	0.3435	8829.388	596.667	5
3N/O	2.04(2)	1(2)					
1N/O	2.18(2)	5(1)	5(3)	0.3199	8221.881	555.613	5
4N/O	2.04(2)	4(2)					
1N/O	2.17(2)	4(2)	3(3)	0.3497	8987.624	607.360	5
3N/O	2.01(2)	1(2)					
2N/O	2.15(2)	2(2)	3(3)	0.3757	9657.405	652.622	5
5N/O	2.03(3)	6(2)					
1N/O	2.17(2)	4(2)	1(3)	0.3910	10049.793	679.139	5

4N/O	2.01(3)	4(3)					
2N/O	2.15(2)	1(2)	1(3)	0.4186	10758.483	727.030	5
3N/O	1.98(3)	2(3)					
3N/O	2.13(3)	0(2)	1(3)	0.4431	11389.418	769.667	5
6N/O	2.02(3)	8(3)					
1N/O	2.16(3)	3(2)	0(4)	0.4359	11204.933	757.200	5
5N/O	2.00(3)	6(3)					
2N/O	2.15(3)	0(2)	-1(4)	0.4638	11919.964	805.520	5
4N/O	1.98(4)	5(3)					
3N/O	2.13(3)	1(3)	-1(4)	0.4880	12542.821	847.611	5

Zn-S(2.2) Zn-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.15(2)	3(1)					
1S	2.28(2)	2(1)	-11(3)	0.1481	3807.810	257.322	5
2S	2.11(2)	3(1)					
2S	2.26(2)	1(1)	-12(3)	0.1702	4373.830	295.572	5
3S	2.15(2)	6(1)					
1S	2.28(2)	1(1)	-13(3)	0.1620	4165.197	281.473	5
4S	2.23(2)	5(1)					
1S	2.06(2)	1(2)	-12(3)	0.2108	5419.354	366.226	5
3S	2.12(2)	6(2)					
2S	2.26(2)	2(1)	-14(3)	0.2031	5219.092	352.693	5
5S	2.23(4)	12(2)					
1S	1.82(8)	21(17)	-5(6)	0.2838	7293.473	492.874	5
4S	2.23(2)	5(1)					
2S	2.07(3)	4(2)	-14(4)	0.2469	6347.223	428.929	5
3S	2.09(3)	7(2)					
3S	2.24(2)	4(2)	-15(4)	0.2525	6489.295	438.530	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.24(4)	12(2)					
2S	1.84(6)	27(14)	-3(7)	0.2725	7003.861	473.303	5
4S	2.23(3)	6(2)	-16(4)	0.2854	7335.016	495.681	5

3S	2.08(3)	8(3)					

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(2)	1(1)					5
1S	2.28(2)	1(1)	0(3)	0.1568	4031.073	272.409	
1N/O	1.96(2)	2(1)					5
2S	2.26(2)	3(1)	-4(3)	0.1678	4312.829	291.450	
2N/O	1.97(3)	2(2)					
2S	2.26(2)	4(1)	-4(3)	0.1986	5104.413	344.943	5
3N/O	2.01(2)	4(2)					
1S	2.28(2)	0(1)	-1(3)	0.1795	4612.858	311.725	5
1N/O	1.94(2)	1(2)					
3S	2.25(2)	6(1)	-6(3)	0.2128	5469.299	369.601	5
1N/O	2.18(2)	4(1)					
4S	2.20(2)	7(1)	-9(3)	0.1625	4176.665	282.248	5
4N/O	2.01(3)	7(2)					
1S	2.28(2)	1(1)	-1(4)	0.2153	5532.990	373.905	5
2N/O	2.12(0.12)	17(51)					
3S	2.25(3)	8(4)	-1(9)	0.2632	6765.288	457.180	5
3N/O	1.98(4)	7(3)					
2S	2.26(2)	4(2)	-4(4)	0.2410	6194.896	418.635	5
5N/O	2.02(4)	11(3)					
1S	2.28(2)	1(2)	-1(4)	0.2518	6473.175	437.440	5
1N/O	2.17(2)	4(1)					
5S	2.19(2)	9(1)	-11(3)	0.1814	4662.769	315.098	5
4N/O	2.20(8)	21(23)					
2S	2.29(2)	5(2)	8(8)	0.2420	6219.896	420.331	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.18(8)	19(60)					
3S	2.26(3)	8(3)	2(12)	0.2530	6502.686	439.434	5
6N/O	2.04(7)	15(4)					
1S	2.27(2)	2(2)	-1(6)	0.2819	7246.931	489.729	5

1N/O	2.17(2)	3(1)					
6S	2.19(2)	11(1)	-12(4)	0.2127	5467.337	369.468	5
5N/O	2.23(6)	25(17)					
2S	2.29(2)	5(1)	9(5)	0.2346	6030.851	407.549	5
2N/O	2.18(2)	2(1)					
5S	2.19(2)	7(1)	-10(3)	0.1615	4150.880	280.506	5
4N/O	2.23(6)	18(24)					
3S	2.28(2)	7(2)	6(7)	0.2392	6148.117	415.474	5
3N/O	2.21(0.46)	21(123)					
4S	2.25(3)	10(3)	-2(22)	0.2629	6757.237	456.636	5

Zn-N(2.0) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(3)	3(2)					5
1Br	2.39(2)	3(1)	-3(5)	0.1430	3675.044	248.350	
1N/O	1.95(3)	0(2)					5
2Br	2.35(2)	7(1)	-13(5)	0.1557	4002.387	270.471	
2N/O	1.98(2)	3(1)					
2Br	2.37(2)	7(1)	-9(4)	0.1061	2727.497	184.317	5
3N/O	2.02(2)	5(1)					
1Br	2.39(1)	4(1)	-2(3)	0.1077	2768.076	187.059	5
1N/O	1.94(2)	0(1)					
3Br	2.35(2)	9(1)	-15(4)	0.1292	3320.702	224.404	5
1N/O	1.93(2)	0(1)					
4Br	2.34(2)	11(1)	-17(4)	0.1202	3089.408	208.774	5
4N/O	2.02(2)	7(1)					
1Br	2.39(1)	4(1)	-3(3)	0.0994	2553.816	172.580	5
2N/O	1.96(2)	3(1)					
3Br	2.36(2)	9(1)	-12(4)	0.0980	2518.285	170.179	5
3N/O	1.99(2)	6(1)					
2Br	2.38(1)	7(1)	-6(3)	0.0855	2198.809	148.590	5
5N/O	2.02(2)	9(2)					
1Br	2.39(1)	4(1)	-3(3)	0.1064	2735.591	184.864	5
1N/O	1.37(0.12)	12(14)					
5Br	2.32(3)	12(1)	-21(6)	0.2352	6046.043	408.576	5

4N/O	2.00(2)	8(1)					
2Br	2.39(1)	7(1)	-6(3)	0.0822	2113.089	142.797	5
2N/O	1.95(2)	4(2)					
4Br	2.36(2)	11(1)	-13(4)	0.1016	2611.218	176.459	5
3N/O	1.98(2)	6(2)					
3Br	2.38(2)	9(1)	-9(4)	0.0873	2244.775	151.696	5
6N/O	2.02(3)	11(2)					
1Br	2.39(1)	4(1)	-4(3)	0.1215	3121.683	210.955	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.01(3)	10(2)					
2Br	2.39(1)	7(1)	-5(3)	0.0888	2283.320	154.301	5
2N/O	1.94(3)	4(2)					
5Br	2.35(2)	12(1)	-15(4)	0.1105	2839.180	191.864	5
4N/O	1.99(3)	9(2)					
3Br	2.38(2)	10(1)	-7(4)	0.0872	2240.668	151.418	5
3N/O	1.97(3)	7(2)					
4Br	2.37(2)	11(1)	-11(4)	0.0973	2501.760	169.062	5

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.02(5)	11(5)					
1S	2.19(4)	7(7)					
1Br	2.39(2)	4(1)	-6(6)	0.0760	1952.574	152.570	7
3N/O	2.00(4)	8(4)					
1S	2.20(6)	7(6)					
1Br	2.39(2)	4(1)	-7(6)	0.0727	1868.540	146.004	7
2N/O	1.97(4)	4(3)					
1S	2.22(7)	4(3)					
1Br	2.39(2)	4(2)	-8(6)	0.0705	1813.084	141.671	7
1N/O	1.93(4)	0(2)					
1S	2.18(4)	1(2)					
1Br	2.38(2)	3(2)	-12(6)	0.0738	1897.430	148.262	7
1S	1.95(3)	0(2)					
1S	2.22(6)	4(4)					
2Br	2.38(2)	9(3)	-9(7)	0.0769	1975.583	154.368	7

2N/O	1.97(2)	3(2)					
1S	2.26(5)	6(6)					
2Br	2.38(1)	8(2)	-7(4)	0.0683	1755.767	137.192	7

Zn-N(2.0) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.04(4)	9(4)					
1Imd	2.15(4)	0(4)	3(4)	0.4273	10981.864	742.126	5
4N/O	2.02(5)	12(7)					
1Imd	2.03(4)	3(3)					
1Imd	2.16(3)	4(3)	1(4)	0.3466	8908.113	696.063	7
3N/O	1.97(9)	19(16)					
1Imd	2.05(3)	12(2)					
1Imd	2.17(2)	11(2)					
1Imd	1.93(3)	9(3)	-1(3)	0.2734	7027.645	650.837	9
2N/O	2.04(7)	7(10)					
1Imd	1.93(5)	8(5)					
1Imd	1.93(4)	14(4)					
1Imd	2.05(4)	16(3)					
1Imd	2.16(3)	13(2)	-3(3)	0.2343	6021.866	684.470	11
1N/O	2.06(8)	1(10)					
1Imd	1.66(0.17)	6(25)					
1Imd	2.05(5)	18(7)					
1Imd	1.93(5)	18(8)					
1Imd	1.82(6)	12(11)					
1Imd	2.16(5)	15(5)	-3(6)	0.1849	4751.982	699.042	13
4N/O	2.05(4)	7(4)					
1Imd	2.16(4)	1(3)	4(4)	0.4120	10590.008	715.645	5
3N/O	2.02(6)	9(7)					
1Imd	2.16(3)	4(3)					
1Imd	2.03(4)	3(4)	2(3)	0.3371	8663.681	676.964	7
2N/O	1.99(9)	12(15)					
1Imd	2.05(3)	12(3)					
1Imd	1.94(3)	8(3)					
1Imd	2.18(3)	11(2)	0(3)	0.2676	6877.470	636.929	9
1N/O	2.06(8)	2(10)					
1Imd	1.94(3)	16(3)					
1Imd	1.83(3)	10(4)					
1Imd	2.05(3)	17(3)					
1Imd	2.17(3)	14(2)	-3(3)	0.2163	5559.774	631.947	11
0N/O			-2(4)	0.2072	5324.726	605.230	11

1Imd	2.17(3)	16(3)					
1Imd	2.06(3)	19(4)					
1Imd	1.95(3)	18(4)					
1Imd	1.84(4)	12(6)					
1Imd	1.68(0.22)	15(34)					
3N/O	2.05(4)	5(4)					
1Imd	2.17(3)	1(3)	5(4)	0.4158	10688.546	722.304	5
2N/O	2.02(6)	6(8)					
1Imd	2.16(3)	5(3)					
1Imd	2.03(5)	3(4)	3(4)	0.3431	8818.987	689.099	7
1N/O	2.01(0.10)	5(13)					
1Imd	2.05(3)	12(2)					
1Imd	1.93(3)	8(3)					
1Imd	2.17(2)	11(2)	0(3)	0.2673	6869.545	636.196	9
0N/O							
1Imd	2.06(2)	18(2)					
1Imd	2.18(2)	15(2)					
1Imd	1.85(2)	11(3)					
1Imd	1.95(2)	17(3)	-3(2)	0.2226	5721.725	529.895	9
2N/O	2.05(4)	2(4)					
1Imd	2.17(4)	2(3)	7(5)	0.4533	11651.030	787.346	5
1N/O	2.01(9)	3(10)					
1Imd	2.02(4)	3(4)					
1Imd	2.16(3)	5(2)	3(4)	0.3769	9687.515	756.964	7
0N/O							
1Imd	1.93(2)	9(2)					
1Imd	2.05(2)	13(2)					
1Imd	2.17(2)	11(2)	1(3)	0.2961	7611.428	594.743	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.98(3)	3(3)					
1S	2.28(1)	0(1)					
1Imd	2.06(3)	0(3)	-1(3)	0.1217	3126.876	244.328	7
1N/O	1.97(2)	2(2)					
1S	2.28(1)	0(1)					
1Imd	2.08(3)	1(2)					
1Imd	2.30(0.23)	19(44)	1(4)	0.0940	2415.666	223.717	9
0N/O							
1S	2.26(2)	1(2)					
1Imd	2.17(3)	7(3)	-1(3)	0.1219	3132.398	290.095	9

1Imd	1.92(3)	6(2)					
1Imd	2.04(3)	9(2)					

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	3(3)					
1S	2.28(1)	0(1)					
1Imd	2.06(3)	0(3)	-1(3)	0.1195	3072.526	240.081	7
1N/O	1.97(2)	2(2)					
1S	2.28(1)	0(1)					
1Imd	2.27(0.21)	19(49)					
1Imd	2.08(3)	1(2)	1(4)	0.0919	2362.216	218.767	9
0N/O							
1S	2.26(2)	1(2)					
1Imd	2.17(3)	7(3)					
1Imd	1.92(3)	6(2)					
1Imd	2.04(3)	9(2)	-1(3)	0.1163	2990.307	276.935	9

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.26(2)	1(2)					
1Imd	2.04(3)	9(2)					
1Imd	2.18(3)	7(3)					
1Imd	1.92(3)	6(2)	-1(2)	0.1126	2893.204	267.943	9

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.63(2)	0(2)					
1Imd	2.03(2)	11(2)					
1Imd	1.92(2)	8(2)					
1Imd	2.15(2)	10(2)	-3(2)	0.1747	4490.073	415.83	9

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.63(2)	0(2)					
1Imd	1.92(2)	8(2)					
1Imd	2.03(2)	11(2)					
1Imd	2.15(2)	10(2)	-3(2)	0.1795	4615.032	427.403	9

Zn-N(2.0) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	4(2)					
1Br	2.40(1)	4(1)					
1Imd	2.07(2)	1(2)	-2(2)	0.0563	1448.352	113.171	7

1N/O	2.00(2)	2(3)					
1Br	2.40(1)	3(0)					
1Imd	2.08(2)	3(1)					
1Imd	1.95(2)	1(1)	-3(1)	0.0228	585.747	54.247	9
0N/O							
1Br	2.39(1)	3(1)					
1Imd	2.02(5)	5(10)					
1Imd	2.11(7)	3(9)					
1Imd	1.91(4)	3(6)	-4(2)	0.0444	1141.713	105.735	9

Zn-N(2.0) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(2)	3(3)					
1Br	2.40(1)	3(0)					
1Imd	2.08(2)	3(1)					
1Imd	1.95(2)	2(1)	-3(2)	0.0248	637.587	59.048	9
0N/O							
1Br	2.40(1)	4(1)					
1Imd	2.11(8)	3(9)					
1Imd	2.02(5)	4(12)					
1Imd	1.92(5)	3(8)	-4(2)	0.0456	1172.707	108.606	9

Zn-N(2.0) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(3)	3(3)					
1Br	2.40(1)	3(0)					
1Imd	1.95(2)	2(1)					
1Imd	2.09(2)	3(1)	-3(2)	0.0267	687.497	63.67	9
0N/O							
1Br	2.40(1)	4(1)					
1Imd	1.92(4)	3(7)					
1Imd	2.11(7)	4(8)					
1Imd	2.02(5)	5(11)	-4(2)	0.0471	1209.595	112.022	9

Zn-N(2.0) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.92(3)	4(2)					
1Br	2.80(4)	5(4)					
1Imd	2.02(3)	8(2)					
1Imd	2.15(3)	8(2)	0(4)	0.2683	6896.056	638.651	9
0N/O							
1Br	2.76(3)	6(3)					
1Imd	1.93(2)	10(2)					
1Imd	2.04(2)	13(2)	-1(3)	0.2249	5780.197	535.31	9

1Imd	2.16(2)	12(2)					

Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	9(3)					
1Br	2.40(1)	4(1)					
1Imd	2.07(1)	3(1)					
1Imd	1.94(1)	2(1)	-5(1)	0.0178	458.767	42.487	9

Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(1)	0(1)					
1Br	2.74(2)	5(1)					
1Imd	1.93(2)	3(2)					
1Imd	2.04(2)	3(2)	-5(2)	0.0605	1555.378	144.045	9

Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	9(3)					
1Br	2.40(1)	4(1)	-5(1)	0.0180	463.71	42.945	9

1Imd	2.07(1)	3(1)					
1Imd	1.94(1)	2(1)					

Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(1)	0(1)					
1Br	2.73(1)	5(1)					
1Imd	1.93(2)	3(2)					
1Imd	2.04(2)	3(2)	-5(2)	0.0574	1476.189	136.711	9

Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	10(3)					
1Br	2.39(1)	4(1)					
1Imd	1.94(1)	2(1)					
1Imd	2.06(1)	3(1)	-5(1)	0.0188	482.779	44.711	9

Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	9(3)					
1Br	2.39(1)	4(1)					
1Imd	1.94(1)	2(1)					
1Imd	2.07(1)	3(1)	-5(1)	0.0183	469.382	43.47	9

Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	9(3)					
1Br	2.40(1)	4(1)					
1Imd	1.94(1)	2(1)					
1Imd	2.07(1)	3(1)	-5(1)	0.0181	465.966	43.154	9

Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(3)	10(3)					
1Br	2.39(1)	4(1)					
1Imd	2.06(1)	3(1)					
1Imd	1.94(1)	2(1)	-5(1)	0.0192	492.284	45.591	9

Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	10(3)	-5(1)	0.0185	476.214	44.103	9

1Br	2.39(1)	4(1)					
1Imd	1.94(1)	2(1)					
1Imd	2.06(1)	3(1)					

Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.91(7)	14(11)					
1Br	2.40(1)	3(1)					
1Imd	1.94(2)	4(1)					
1Imd	2.07(2)	5(1)	-4(2)	0.0540	1387.187	128.469	9

Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.91(7)	14(11)					
1Br	2.40(1)	3(1)					
1Imd	2.07(2)	5(1)					
1Imd	1.94(2)	4(1)	-4(2)	0.0550	1413.022	130.861	9

Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.94(6)	13(10)					
1Br	2.40(1)	3(1)					
1Imd	1.94(2)	4(1)					
1Imd	2.07(2)	5(1)	-4(2)	0.0520	1335.94	123.723	9

Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.93(7)	14(10)					
1Br	2.40(1)	3(1)					
1Imd	1.94(2)	4(1)					
1Imd	2.07(2)	5(1)	-4(2)	0.0529	1360.135	125.963	9

Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.92(7)	14(10)					
1Br	2.40(1)	3(1)					
1Imd	1.94(2)	4(1)					
1Imd	2.07(2)	5(1)	-4(2)	0.0540	1386.784	128.431	9

Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.62(2)	1(2)					
1Br	3.07(0.55)	26(77)					
1Imd	2.10(2)	6(2)					
1Imd	1.96(2)	5(2)	-4(4)	0.2550	6554.555	607.024	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.94(2)	0(2)					
1S	2.25(3)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0259	665.048	61.591	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(1)					
1S	2.25(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0247	634.614	58.772	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(1)					
1S	2.25(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	0(1)	-4(2)	0.0239	613.233	56.792	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(1)					
1S	2.25(2)	4(1)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	0(1)	-4(2)	0.0233	599.059	55.479	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(2)					
1S	2.26(3)	4(2)					
1Br	2.39(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0271	695.297	64.392	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(2)					
1S	2.26(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0258	663.242	61.423	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(1)					
1S	2.26(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0249	640.338	59.302	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(1)					
1S	2.26(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0243	624.857	57.869	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(2)					
1S	2.26(3)	5(2)					
1Br	2.39(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0281	722.239	66.887	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(2)					
1S	2.26(3)	4(2)					
1Br	2.39(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0268	689.081	63.816	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(2)					
1S	2.26(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0259	665.22	61.607	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(1)					
1S	2.26(2)	4(2)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	1(1)	-4(2)	0.0252	648.964	60.101	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(2)					
1S	2.26(3)	5(2)					
1Br	2.39(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0291	748.593	69.328	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	0(2)					
1S	2.26(3)	4(2)					
1Br	2.39(1)	6(1)					
1Imd	2.05(2)	1(2)	-4(2)	0.0278	714.271	66.149	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	1(2)					
1S	2.75(4)	4(3)					
1Br	2.39(2)	3(1)					
1Imd	2.08(3)	2(2)	-2(4)	0.0831	2134.811	197.707	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	1(2)					
1S	2.75(4)	3(3)					
1Br	2.40(2)	3(1)					
1Imd	2.08(3)	2(2)	-2(4)	0.0842	2163.258	200.342	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(3)	1(2)					
1S	2.75(4)	5(4)					
1Br	2.39(2)	3(1)					
1Imd	2.08(3)	1(2)	-2(4)	0.0835	2146.94	198.83	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(3)	1(2)					
1S	2.75(4)	4(3)					
1Br	2.39(2)	3(1)					
1Imd	2.08(3)	1(2)	-2(4)	0.0844	2169.096	200.882	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	1(2)					
1S	2.75(4)	4(3)					
1Br	2.39(2)	2(1)					
1Imd	2.08(3)	2(2)	-2(4)	0.0852	2190.959	202.907	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(3)	7(2)					
1S	2.73(6)	7(5)					
1Br	2.69(4)	4(4)					
1Imd	1.96(3)	5(2)	-5(5)	0.2191	5631.849	521.571	9

Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(5)	7(4)					
2Br	2.38(2)	8(1)					
1Imd	1.98(2)	1(2)	-7(4)	0.0685	1761.296	137.624	7

Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(4)	6(4)					
2Br	2.38(2)	8(1)					
1Imd	1.98(2)	1(2)	-7(4)	0.0690	1774.033	138.620	7

Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(4)	6(3)					
2Br	2.39(2)	9(1)					
1Imd	1.98(2)	1(2)	-7(4)	0.0698	1794.067	140.185	7

Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(4)	6(3)					
2Br	2.39(2)	9(1)					
1Imd	1.98(2)	1(2)	-7(4)	0.0707	1817.053	141.981	7

Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(5)	7(4)					
2Br	2.38(2)	8(1)					
1Imd	1.98(2)	1(2)	-7(4)	0.0686	1763.484	137.795	7

Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(4)	7(4)					
2Br	2.38(2)	9(1)					
1Imd	1.98(2)	1(2)	-7(4)	0.0689	1769.838	138.292	7

Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(4)	6(4)					
2Br	2.38(2)	9(2)					
1Imd	1.98(2)	1(2)	-7(4)	0.0694	1784.590	139.444	7

Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(4)	6(4)					
2Br	2.39(2)	9(2)					
1Imd	1.98(2)	1(2)	-7(4)	0.0702	1803.183	140.897	7

Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(5)	7(4)					
2Br	2.38(2)	8(1)					
1Imd	1.98(2)	1(2)	-7(4)	0.0685	1761.691	137.655	7

Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(4)	7(4)					
2Br	2.38(2)	9(2)					
1Imd	1.98(2)	1(2)	-7(4)	0.0686	1763.594	137.804	7

Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(4)	6(4)					
2Br	2.39(2)	9(2)					
1Imd	1.98(2)	1(2)	-7(4)	0.0697	1790.434	139.901	7

Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(5)	7(4)					
2Br	2.38(2)	8(2)					
1Imd	1.98(2)	1(2)	-7(4)	0.0685	1760.779	137.584	7

Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(4)	7(4)					
2Br	2.38(2)	9(2)					
1Imd	1.98(2)	1(2)	-7(4)	0.0684	1758.851	137.433	7

Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(4)	6(4)					
2Br	2.38(2)	9(2)					
1Imd	1.98(2)	1(1)	-7(4)	0.0687	1767.067	138.075	7

Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.85(9)	12(14)					
2Br	2.38(2)	7(1)					
1Imd	1.99(3)	1(2)	-7(5)	0.1508	3876.520	302.904	7

Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	1.70(5)	19(6)					
2Br	2.40(1)	7(1)					
1Imd	2.03(2)	1(2)	-3(3)	0.1030	2647.166	206.845	7

Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(4)	6(4)					
2Br	2.38(2)	9(2)					
1Imd	1.98(2)	1(1)	-7(4)	0.0682	1753.198	136.992	7

Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(4)	6(4)					
2Br	2.38(2)	9(2)					
1Imd	1.98(2)	1(1)	-7(4)	0.0687	1764.941	137.909	7

Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br	2.39(1)	7(1)					
1Imd	1.94(2)	3(1)					
1Imd	2.07(2)	3(1)	-5(2)	0.0630	1620.104	126.592	7

Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br	2.79(4)	11(4)					
1Imd	2.13(3)	6(2)					
1Imd	2.00(3)	5(2)	1(4)	0.3890	9998.953	781.299	7

Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.39(1)	3(1)					
1Br	2.46(0.11)	19(15)					
1Imd	1.94(2)	3(2)					
1Imd	2.07(2)	4(1)	-4(2)	0.0576	1479.26	136.996	9

Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.39(1)	3(1)					
1Br	2.47(0.11)	19(16)					
1Imd	2.07(2)	4(1)					
1Imd	1.94(2)	3(2)	-4(2)	0.0585	1504.604	139.343	9

Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.39(1)	3(1)					
1Br	2.48(0.10)	19(16)					
1Imd	2.07(2)	4(1)					
1Imd	1.94(2)	3(2)	-4(2)	0.0597	1534.288	142.092	9

Zn-S(2.2) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(1)	7(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	1(1)	-6(2)	0.0260	668.528	61.913	9

Zn-S(2.3) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.01(2)	0(1)	-6(2)	0.0277	710.901	65.837	9

Zn-S(2.4) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.01(2)	0(2)	-6(2)	0.0287	737.457	68.297	9

Zn-S(2.5) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.29(3)	4(3)					
1Br	2.39(1)	6(2)					
1Br	1.89(2)	11(2)					
1Imd	2.04(2)	1(2)	-3(3)	0.0385	988.847	91.578	9

Zn-S(2.6) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	0(2)	-7(3)	0.0295	758.973	70.289	9

Zn-S(2.2) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	1(1)	-6(2)	0.0265	680.129	62.987	9

Zn-S(2.3) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.01(2)	0(1)	-6(2)	0.0279	718.173	66.511	9

Zn-S(2.4) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	1(1)					
1Imd	2.01(2)	0(1)	-6(2)	0.0289	743.373	68.844	9

Zn-S(2.5) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	1(1)					
1Imd	2.00(2)	0(2)	-7(3)	0.0306	786.134	72.805	9

Zn-S(2.6) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	1(1)					
1Imd	2.00(2)	0(2)	-7(3)	0.0298	765.06	70.853	9

Zn-S(2.2) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(4)	0(2)					
1Br	2.41(4)	3(2)					
1Br	2.65(7)	9(7)					
1Imd	1.95(4)	0(3)	-8(5)	0.0618	1588.961	147.155	9

Zn-S(2.3) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.29(3)	3(3)					
1Br	2.40(1)	6(2)					
1Br	1.90(2)	11(2)					
1Imd	2.04(2)	1(2)	-2(3)	0.0371	954.184	88.368	9

Zn-S(2.4) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(4)	0(2)					
1Br	2.41(4)	3(3)					
1Br	2.65(6)	9(7)					
1Imd	1.95(4)	0(3)	-9(5)	0.0633	1626.431	150.625	9

Zn-S(2.5) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(4)	0(2)					
1Br	2.41(4)	3(3)					
1Br	2.65(1)	8(6)					
1Imd	1.94(4)	0(2)	-9(5)	0.0632	1623.786	150.38	9

Zn-S(2.6) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.51(3)	4(1)					
1Br	2.08(3)	0(1)					
1Br	2.21(3)	2(1)					
1Imd	1.69(6)	6(6)	-48(7)	0.0678	1743.552	161.472	9

Zn-S(2.2) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(1)	7(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)	-6(2)	0.0258	664.171	61.51	9

1Imd	2.00(2)	1(1)					

Zn-S(2.3) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	7(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	0(1)	-6(2)	0.0271	696.703	64.522	9

Zn-S(2.4) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	0(1)	-6(2)	0.0280	719.677	66.65	9

Zn-S(2.5) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	0(2)	-7(2)	0.0296	761.227	70.498	9

Zn-S(2.6) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	0(2)	-7(2)	0.0288	740.947	68.62	9

Zn-S(2.2) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(4)	0(2)					
1Br	2.42(4)	3(2)					
1Br	2.65(6)	8(6)					
1Imd	1.95(4)	0(2)	-8(5)	0.0607	1561.277	144.591	9

Zn-S(2.3) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(4)	0(2)					
1Br	2.42(4)	3(3)					
1Br	2.65(6)	8(6)					
1Imd	1.95(4)	0(2)	-9(5)	0.0618	1589.48	147.203	9

Zn-S(2.4) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(4)	0(2)					
1Br	2.42(4)	3(3)	-9(5)	0.0622	1598.897	148.075	9

1Br	2.65(6)	8(6)					
1Imd	1.95(4)	0(2)					

Zn-S(2.5) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(1)					
1Br	2.19(2)	2(1)					
1Br	2.40(1)	0(1)					
1Imd	2.00(2)	0(2)	-7(2)	0.0298	766.634	70.999	9

Zn-S(2.6) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.86(3)	0(2)					
1Br	2.31(3)	2(1)					
1Br	2.45(3)	2(1)					
1Imd	1.95(3)	3(1)	-9(4)	0.0797	2048.641	189.727	9

Zn-S(2.2) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(3)	1(2)					
1Br	2.65(5)	6(5)					
1Br	2.43(4)	3(3)					
1Imd	1.94(3)	1(2)	-8(4)	0.0585	1503.694	139.259	9

Zn-S(2.3) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(1)	7(1)					
1Br	2.39(1)	0(1)					
1Br	2.19(2)	2(1)					
1Imd	2.00(2)	0(1)	-6(2)	0.0259	665.278	61.612	9

Zn-S(2.4) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(4)	0(2)					
1Br	2.42(4)	3(3)					
1Br	2.65(6)	7(6)					
1Imd	1.94(4)	0(2)	-9(5)	0.0611	1571.654	145.553	9

Zn-S(2.5) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.29(3)	3(3)					
1Br	2.40(1)	7(2)					
1Br	1.89(2)	12(2)					
1Imd	2.04(2)	1(2)	-3(3)	0.0379	973.527	90.159	9

Zn-S(2.6) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.86(3)	0(2)	-9(4)	0.0805	2070.192	191.723	9

1Br	2.32(3)	2(1)					
1Br	2.46(3)	2(1)					
1Imd	1.95(3)	3(1)					

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	1.98(5)	9(5)					
1S	2.28(2)	0(1)					
1Imd	2.03(3)	1(3)	-2(3)	0.1552	3990.271	311.792	7
2N/O	1.96(4)	5(3)					
1S	2.26(2)	1(1)					
1Imd	2.04(4)	1(3)					
1Imd	2.47(3)	0(3)	-4(3)	0.0979	2516.228	233.030	9
1N/O	1.96(3)	3(2)					
1S	2.27(2)	1(1)					
1Imd	2.08(3)	2(3)					
1Imd	2.50(4)	0(5)					
1Imd	2.27(7)	1(7)	1(4)	0.0727	1867.640	212.284	9

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	1.98(5)	9(5)					
1S	2.28(2)	0(1)					
1Imd	2.03(3)	1(3)	-2(3)	0.1521	3909.045	305.445	7
2N/O	1.96(4)	5(4)					
1S	2.27(2)	1(1)					
1Imd	2.47(3)	0(3)					
1Imd	2.03(4)	1(3)	-4(3)	0.0974	2504.430	231.938	9
1N/O	1.96(3)	3(2)					
1S	2.27(2)	1(1)					
1Imd	2.26(8)	1(8)					
1Imd	2.07(3)	2(3)					
1Imd	2.50(4)	0(5)	0(4)	0.0741	1904.869	216.515	9

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	3(2)					
1S	2.27(2)	0(2)					
1Imd	2.50(4)	0(5)					
1Imd	2.07(3)	2(3)					
1Imd	2.26(8)	2(9)	0(4)	0.0752	1933.492	219.769	9

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(0.12)	10(21)	-3(2)	0.1435	3689.717	419.388	9

1S	2.63(2)	1(2)					
1Imd	2.16(3)	10(3)					
1Imd	2.04(3)	11(3)					
1Imd	1.93(3)	8(3)					

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(0.12)	9(21)					
1S	2.63(2)	1(2)					
1Imd	2.04(3)	11(3)					
1Imd	1.93(3)	8(3)					
1Imd	2.16(3)	10(3)	-3(2)	0.1477	3797.486	431.638	9

Zn-N(2.0) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.00(2)	7(2)					
1Br	2.40(1)	4(1)					
1Imd	2.07(2)	1(2)	-2(2)	0.0193	497.017	56.493	7
2N/O	1.99(2)	8(3)					
1Br	2.40(1)	4(0)					
1Imd	1.96(2)	1(2)					
1Imd	2.09(1)	2(1)	-3(1)	0.0196	503.883	46.665	9
1N/O	2.00(2)	2(3)					
1Br	2.39(1)	3(1)					
1Imd	2.08(2)	3(1)					
1Imd	1.95(2)	2(2)					
1Imd	1.90(0.13)	19(29)	-5(2)	0.0465	1195.759	93.434	11

Zn-N(2.0) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.00(2)	7(2)					
1Br	2.40(1)	4(1)					
1Imd	2.07(2)	1(2)	-2(2)	0.0489	1257.311	98.244	7
2N/O	1.99(2)	8(3)					
1Br	2.40(1)	4(0)					
1Imd	1.97(2)	1(2)					
1Imd	2.09(1)	3(1)	-3(1)	0.0207	532.166	49.284	9
1N/O	2.00(2)	2(3)					
1Br	2.39(1)	3(1)					
1Imd	1.95(2)	2(2)					
1Imd	2.08(2)	3(2)					
1Imd	1.90(0.13)	18(28)	-5(2)	0.0210	540.926	61.484	11

Zn-N(2.0) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2N/O	1.99(2)	8(3)					
1Br	2.40(1)	4(0)					
1Imd	2.09(2)	3(1)					
1Imd	1.97(2)	1(2)	-3(1)	0.0220	565.507	52.372	9
1N/O	2.00(3)	3(3)					
1Br	2.40(1)	3(1)					
1Imd	1.95(2)	2(2)					
1Imd	2.08(2)	3(2)					
1Imd	1.90(0.13)	18(29)	-5(2)	0.0228	586.236	66.634	11

Zn-N(2.0) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(6)	6(9)					
1Br	2.79(5)	8(5)					
1Imd	2.15(4)	6(2)					
1Imd	2.02(5)	5(3)	1(4)	0.2775	7132.450	660.543	9
1N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	9(3)					
1Br	2.40(1)	4(1)					
1Imd	2.05(1)	6(2)					
1Imd	1.93(1)	4(1)					
1Imd	2.17(2)	2(3)	-3(1)	0.0107	275.466	31.311	11

Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	9(3)					
1Br	2.40(1)	4(1)					
1Imd	1.93(1)	4(1)					
1Imd	2.17(2)	2(3)					
1Imd	2.05(1)	6(2)	-3(1)	0.0110	282.728	32.136	11

Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	9(3)					
1Br	2.40(1)	4(1)					
1Imd	2.05(1)	6(2)					
1Imd	2.17(2)	2(3)					
1Imd	1.93(1)	4(1)	-3(1)	0.0107	273.787	31.120	11

Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	9(3)					
1Br	2.40(1)	4(1)					
1Imd	1.93(1)	4(1)					
1Imd	2.17(2)	2(3)					
1Imd	2.05(1)	6(2)	-3(1)	0.0108	277.452	31.536	11

Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	10(3)					
1Br	2.40(1)	4(1)					
1Imd	1.93(1)	4(1)					
1Imd	2.17(2)	2(3)					
1Imd	2.05(1)	6(2)	-3(1)	0.0106	272.867	31.015	11

Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	10(3)					
1Br	2.40(1)	4(1)					
1Imd	1.93(1)	4(1)					
1Imd	2.17(2)	2(3)					
1Imd	2.05(1)	6(2)	-3(1)	0.0106	272.340	30.955	11

Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	10(3)					
1Br	2.39(1)	4(1)					
1Imd	1.93(1)	4(1)					
1Imd	2.05(1)	6(2)					
1Imd	2.17(2)	3(3)	-3(1)	0.0107	274.613	31.214	11

Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.63(2)	0(2)					
1Br	3.20(4)	6(3)					
1Imd	2.15(2)	11(2)					
1Imd	2.03(2)	12(2)					
1Imd	1.92(2)	9(2)	-3(2)	0.1433	3683.649	418.699	11

Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.94(6)	13(8)					
1Br	2.40(1)	3(1)					
1Imd	2.02(5)	5(11)					
1Imd	2.11(7)	4(8)					
1Imd	1.91(4)	3(7)	-4(2)	0.0332	852.840	96.937	11

Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.93(6)	13(9)					
1Br	2.40(1)	3(1)					
1Imd	2.01(5)	5(11)					
1Imd	1.92(4)	3(7)					
1Imd	2.11(7)	4(8)	-4(2)	0.0338	867.645	98.620	11

Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.93(6)	13(9)					
1Br	2.40(1)	4(1)					
1Imd	2.02(4)	5(9)					
1Imd	1.91(4)	3(6)					
1Imd	2.11(6)	4(7)	-4(2)	0.0345	886.625	100.777	11

Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.63(2)	0(2)					
1Br	3.20(4)	6(4)					
1Imd	2.15(2)	11(2)					
1Imd	2.03(2)	12(2)					
1Imd	1.92(2)	9(2)	-3(2)	0.1484	3814.395	433.560	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	5(4)					
1S	2.23(4)	15(5)					
1Br	2.40(1)	4(0)					
1Imd	2.08(1)	2(1)					
1Imd	1.95(2)	0(1)	-4(1)	0.0099	253.998	28.870	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	7(3)					
1S	2.25(4)	8(4)					
1Br	2.39(1)	5(1)					
1Imd	2.04(3)	3(2)	-4(2)	0.0325	835.056	77.335	9
1N/O	1.99(3)	6(4)					
1S	2.24(3)	14(5)					
1Br	2.40(1)	4(0)					
1Imd	2.09(1)	2(1)					
1Imd	1.96(2)	1(1)	-4(1)	0.0099	255.296	29.018	11
0N/O							
1S	2.22(2)	9(3)					
1Br	2.40(1)	4(1)					
1Imd	2.17(2)	2(3)					
1Imd	1.93(1)	4(1)					
1Imd	2.05(1)	6(2)	-3(1)	0.0107	275.466	31.311	11

Zn-N(2.2) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(4)	15(6)					
1S	2.23(1)	4(0)					
1Br	2.40(1)	2(1)					
1Imd	2.08(1)	1(1)					
1Imd	1.95(4)	6(5)	-4(1)	0.0101	260.279	29.584	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	6(4)					
1S	2.24(3)	13(4)					
1Br	2.40(1)	4(0)					
1Imd	2.09(1)	2(1)					
1Imd	1.96(1)	1(1)	-4(1)	0.0102	261.513	29.725	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	3(2)					
1S	2.26(1)	1(1)					
1Br	2.79(2)	6(2)					
1Imd	2.17(5)	1(6)					
1Imd	2.04(2)	4(2)	-1(2)	0.0358	919.648	104.531	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(3)	5(3)					
1S	2.24(4)	15(5)					
1Br	2.39(1)	4(0)	-4(1)	0.0096	246.122	27.975	11

1Imd	2.08(1)	2(1)					
1Imd	1.95(2)	0(1)					

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	5(4)					
1S	2.24(3)	14(5)					
1Br	2.40(1)	4(0)					
1Imd	1.96(1)	0(1)					
1Imd	2.08(1)	2(1)	-4(1)	0.0096	245.725	27.930	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	6(4)					
1S	2.24(3)	13(4)					
1Br	2.40(1)	4(0)					
1Imd	1.96(1)	1(1)					
1Imd	2.09(1)	2(1)	-4(1)	0.0097	250.361	28.457	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	3(2)					
1S	2.27(1)	0(1)					
1Br	2.79(2)	6(2)					
1Imd	2.17(5)	1(6)					
1Imd	2.04(2)	4(2)	-1(2)	0.0353	907.490	103.149	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(3)	5(3)					
1S	2.24(4)	16(5)					
1Br	2.39(1)	4(0)					
1Imd	2.08(1)	2(1)					
1Imd	1.95(2)	0(1)	-4(1)	0.0094	241.114	27.406	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	5(3)					
1S	2.25(3)	15(5)					
1Br	2.40(1)	4(0)					
1Imd	2.08(1)	2(1)					
1Imd	1.95(1)	0(1)	-4(1)	0.0093	239.621	27.236	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	6(3)					
1S	2.25(3)	14(4)					
1Br	2.40(1)	4(0)	-4(1)	0.0095	243.262	27.650	11

1Imd	2.08(1)	2(1)					
1Imd	1.96(1)	1(1)					

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	3(2)					
1S	2.27(1)	0(1)					
1Br	2.79(2)	7(2)					
1Imd	2.04(2)	4(2)					
1Imd	2.17(5)	1(6)	-1(2)	0.0353	906.523	103.039	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(3)	5(3)					
1S	2.24(3)	17(5)					
1Br	2.39(1)	4(0)					
1Imd	1.95(2)	0(1)					
1Imd	2.08(1)	2(1)	-4(1)	0.0092	236.967	26.935	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	5(2)					
1S	2.25(3)	15(5)					
1Br	2.40(1)	4(0)					
1Imd	1.95(1)	1(1)					
1Imd	2.08(1)	2(1)	-4(1)	0.0091	234.599	26.665	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	2(3)					
1S	2.86(6)	16(10)					
1Br	2.40(1)	3(0)					
1Imd	1.94(2)	2(1)					
1Imd	2.08(2)	3(1)	-3(2)	0.0195	500.736	56.916	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(2)	2(3)					
1S	2.89(8)	20(13)					
1Br	2.40(1)	3(0)					
1Imd	2.08(2)	3(1)					
1Imd	1.95(2)	2(1)	-3(2)	0.0177	455.091	51.727	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	2(3)					
1S	2.89(7)	19(12)					
1Br	2.40(1)	3(0)	-3(2)	0.0188	482.233	54.813	11

1Imd	2.08(2)	3(1)					
1Imd	1.95(2)	2(1)					

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	2(3)					
1S	2.88(6)	17(11)					
1Br	2.40(1)	3(0)					
1Imd	2.08(2)	3(1)					
1Imd	1.95(2)	2(1)	-3(2)	0.0197	507.508	57.685	11

Zn-N(2.0) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	3(3)					
2Br	2.40(1)	7(1)					
1Imd	2.10(2)	2(2)					
1Imd	1.97(2)	1(2)	-3(2)	0.0260	675.602	62.568	9

Zn-N(2.0) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	3(3)					
2Br	2.40(1)	7(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.10(2)	2(2)	-3(2)	0.0293	751.998	69.643	9

Zn-N(2.0) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	3(3)					
2Br	2.40(1)	8(1)					
1Imd	1.98(2)	1(2)					
1Imd	2.10(2)	2(2)	-3(2)	0.0323	831.028	76.962	9

Zn-N(2.0) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.15(3)	6(2)					
2Br	2.76(3)	7(2)					
1Imd	1.96(3)	5(4)					
1Imd	2.06(4)	5(4)	-2(4)	0.2944	7566.471	700.739	9

Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(4)	12(7)					
2Br	2.39(1)	8(1)					
1Imd	1.94(2)	1(2)					
1Imd	2.07(2)	1(2)	-5(2)	0.0306	786.007	72.793	9

Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(4)	11(6)					
2Br	2.39(1)	8(1)					
1Imd	1.94(2)	1(2)					
1Imd	2.07(3)	1(2)	-5(2)	0.0325	835.886	77.412	9

Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(1)	0(1)					
2Br	2.75(2)	10(2)					
1Imd	1.94(2)	3(2)					
1Imd	2.05(2)	4(2)	-4(2)	0.0826	2121.941	196.515	9

Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(4)	12(7)					
2Br	2.39(1)	8(1)					
1Imd	2.06(2)	2(2)					
1Imd	1.94(2)	1(2)	-5(2)	0.0298	766.185	70.957	9

Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(4)	11(7)					
2Br	2.39(1)	8(1)					
1Imd	1.94(2)	1(2)					
1Imd	2.06(2)	1(2)	-5(2)	0.0305	782.774	72.493	9

Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.27(1)	0(1)					
2Br	2.75(2)	10(2)					
1Imd	1.94(2)	3(2)					
1Imd	2.05(2)	4(2)	-4(2)	0.0786	2020.308	187.103	9

Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.28(1)	0(1)					
2Br	2.74(2)	10(2)					
1Imd	2.05(2)	4(2)					
1Imd	1.94(2)	3(2)	-4(2)	0.0761	1954.943	181.049	9

Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.29(3)	10(6)					
2Br	2.39(1)	8(1)					
1Imd	2.06(2)	1(2)					
1Imd	1.94(2)	1(2)	-5(2)	0.0307	789.57	73.123	9

Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.91(3)	8(4)					
2Br	2.39(1)	7(1)					
1Imd	2.06(2)	4(1)					
1Imd	1.94(1)	3(1)	-5(2)	0.0365	938.286	86.896	9

Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.30(3)	10(6)					
2Br	2.39(1)	8(1)					
1Imd	2.06(2)	1(2)					
1Imd	1.94(2)	1(2)	-5(2)	0.0301	774.621	71.738	9

Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br	2.39(1)	7(1)					
1Imd	2.09(9)	2(5)					
1Imd	1.96(0.13)	1(6)					
1Imd	1.96(0.28)	7(37)	-5(2)	0.0467	1201.056	111.231	9

Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br	2.40(1)	7(1)					
1Imd	1.96(0.24)	7(34)					
1Imd	2.09(8)	2(4)					
1Imd	1.97(0.11)	1(5)	-5(2)	0.0500	1283.905	118.904	9

Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br	2.40(1)	8(1)					
1Imd	1.97(0.11)	1(5)					
1Imd	2.09(8)	2(5)					
1Imd	1.96(0.24)	7(34)	-5(2)	0.0532	1367.984	126.69	9

Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2Br	2.78(3)	11(4)					
1Imd	2.05(2)	13(2)					
1Imd	2.17(2)	12(2)					
1Imd	1.93(2)	10(2)	0(3)	0.2267	5826.538	539.602	9

Zn-N(2.0) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(2)	0(3)					
1Br	2.38(1)	3(1)					
1Br	2.51(4)	11(7)					
1Imd	1.93(3)	0(2)					
1Imd	2.08(2)	2(1)	-4(2)	0.0165	423.354	48.120	11

Zn-N(2.0) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(2)	0(3)					
1Br	2.39(1)	3(1)					
1Br	2.51(4)	12(7)					
1Imd	2.08(2)	2(1)					
1Imd	1.93(3)	0(2)	-4(2)	0.0170	437.830	49.766	11

Zn-N(2.0) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(2)	0(3)					
1Br	2.39(1)	3(1)					
1Br	2.52(4)	13(7)					
1Imd	2.52(3)	0(2)					
1Imd	2.08(2)	2(1)	-4(2)	0.0175	449.664	51.111	11

Zn-N(2.0) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(2)	0(3)					
1Br	2.39(1)	2(1)					
1Br	2.52(4)	10(6)					
1Imd	2.08(2)	3(1)					
1Imd	1.93(3)	0(2)	-4(2)	0.0174	448.319	50.958	11

Zn-N(2.0) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(2)	0(3)					
1Br	2.39(1)	3(1)					
1Br	2.52(4)	11(6)					
1Imd	2.08(2)	3(1)					
1Imd	1.93(3)	0(2)	-4(2)	0.0180	461.679	52.476	11

Zn-N(2.0) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(2)	1(3)					
1Br	2.39(1)	2(1)					
1Br	2.52(3)	10(6)					
1Imd	2.08(2)	3(1)					
1Imd	1.93(3)	0(2)	-4(2)	0.0184	474.055	53.883	11

Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.39(1)	4(1)					
1Br	2.49(0.16)	24(27)					
1Imd	2.11(8)	3(12)					
1Imd	1.91(4)	3(6)					
1Imd	2.02(6)	4(11)	-3(2)	0.0422	1083.458	123.150	11

Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.39(1)	3(1)					
1Br	2.52(0.22)	27(36)					
1Imd	1.91(4)	3(7)					
1Imd	2.11(9)	3(12)					
1Imd	2.02(6)	4(12)	-4(2)	0.0426	1095.137	124.478	11

Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.39(1)	3(1)					
1Br	2.55(0.26)	29(42)					
1Imd	2.11(0.10)	3(13)					
1Imd	2.02(7)	4(13)					
1Imd	1.91(5)	3(8)	-4(2)	0.0429	1102.594	125.325	11

Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.39(1)	4(1)					
1Br	2.52(0.19)	26(31)					
1Imd	1.97(0.69)	3(61)					
1Imd	1.97(0.48)	0(20)					
1Imd	2.09(0.15)	3(6)	-4(2)	0.0434	1116.143	126.865	11

Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.4(1)	4(1)					
1Br	2.54(0.22)	27(34)					
1Imd	2.11(0.12)	3(14)					
1Imd	1.92(6)	2(9)					
1Imd	2.02(8)	4(18)	-4(2)	0.0436	1121.815	127.510	11

Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1Br	2.40(1)	4(1)					
1Br	2.54(0.19)	25(29)					
1Imd	1.92(6)	2(9)					
1Imd	2.11(0.11)	3(13)					
1Imd	2.02(7)	4(16)	-4(2)	0.0446	1146.979	130.370	11

Zn-S(2.2) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	4(2)					
1Br	2.20(2)	0(2)					
1Br	2.40(1)	1(1)					
1Imd	2.07(2)	1(3)					
1Imd	1.96(2)	0(4)	-5(1)	0.0082	209.823	23.849	11

Zn-S(2.3) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	4(2)					
1Br	2.20(2)	0(3)					
1Br	2.40(1)	1(1)					
1Imd	1.95(2)	0(3)					
1Imd	2.07(2)	1(2)	-5(1)	0.0080	204.730	23.270	11

Zn-S(2.4) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	4(3)					
1Br	2.21(2)	0(3)					
1Br	2.40(1)	2(1)					
1Imd	1.95(2)	0(3)					
1Imd	2.07(2)	2(2)	-5(1)	0.0083	212.667	24.173	11

Zn-S(2.5) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(3)					
1Br	2.21(2)	1(3)					
1Br	2.40(1)	2(1)					
1Imd	1.94(2)	1(2)					
1Imd	2.07(2)	2(2)	-5(1)	0.0091	233.146	26.500	11

Zn-S(2.6) Zn-Br(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(3)					
1Br	2.22(2)	1(3)					
1Br	2.40(1)	2(1)					
1Imd	2.07(1)	2(1)					
1Imd	1.94(2)	1(2)	-5(1)	0.0092	236.794	26.915	11

Zn-S(2.2) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	5(2)					
1Br	2.20(2)	0(2)					
1Br	2.40(1)	1(1)					
1Imd	2.07(3)	1(4)					
1Imd	1.96(3)	0(4)	-5(1)	0.0085	218.308	24.814	11

Zn-S(2.3) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	4(2)					
1Br	2.20(2)	0(3)					
1Br	2.40(1)	1(1)					
1Imd	1.95(2)	0(4)					
1Imd	2.07(2)	1(3)	-5(1)	0.0082	211.443	24.033	11

Zn-S(2.4) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	4(3)					
1Br	2.20(2)	0(3)					
1Br	2.40(1)	2(1)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(2)	0(3)	-5(1)	0.0085	218.194	24.801	11

Zn-S(2.5) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(3)					
1Br	2.21(2)	1(3)					
1Br	2.40(1)	2(1)					
1Imd	1.95(2)	1(3)					
1Imd	2.07(2)	2(2)	-5(1)	0.0093	239.744	27.250	11

Zn-S(2.6) Zn-Br(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(3)					
1Br	2.21(2)	1(3)					
1Br	2.40(1)	2(1)					
1Imd	2.07(2)	2(1)					
1Imd	1.94(2)	1(2)	-5(1)	0.0094	241.559	27.457	11

Zn-S(2.2) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(3)					
1Br	2.40(1)	4(1)					
1Br	2.67(3)	14(5)					
1Imd	1.94(1)	2(1)					
1Imd	2.07(1)	3(1)	-5(1)	0.0129	332.228	37.762	11

Zn-S(2.3) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	5(3)					
1Br	2.40(1)	4(1)					
1Br	2.67(3)	13(5)					
1Imd	2.06(1)	3(1)					
1Imd	1.93(1)	2(1)	-5(1)	0.0142	363.745	41.345	11

Zn-S(2.4) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	7(3)					
1Br	2.40(1)	4(1)					
1Br	2.67(3)	14(5)					
1Imd	2.06(1)	3(1)					
1Imd	1.94(1)	2(1)	-5(1)	0.0138	354.979	40.348	11

Zn-S(2.5) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	2(4)					
1Br	2.40(1)	1(1)					
1Br	2.22(2)	2(4)					
1Imd	2.07(1)	2(1)					
1Imd	1.94(1)	1(1)	-5(1)	0.0094	241.571	27.458	11

Zn-S(2.6) Zn-Br(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.93(0.16)	24(29)					
1Br	2.39(1)	3(1)					
1Br	3.10(5)	10(5)					
1Imd	2.07(2)	5(1)					
1Imd	1.94(2)	4(1)	-4(2)	0.0448	1150.481	130.768	11

Zn-S(2.2) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.3) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	4(3)					
1Br	2.40(1)	1(1)					
1Br	2.20(2)	0(3)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(2)	0(3)	-5(1)	0.0084	216.227	24.577	11

Zn-S(2.4) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	4(3)					
1Br	2.20(2)	0(3)					
1Br	2.40(1)	2(1)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(2)	0(3)	-5(1)	0.0086	221.902	25.222	11

Zn-S(2.5) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	3(3)					
1Br	2.21(2)	1(4)					
1Br	2.40(1)	2(1)					
1Imd	2.07(2)	2(2)					
1Imd	1.95(2)	1(3)	-5(1)	0.0095	243.280	27.652	11

Zn-S(2.6) Zn-Br(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	3(4)					
1Br	2.21(2)	1(4)					
1Br	2.40(1)	2(1)					
1Imd	2.07(2)	2(2)					
1Imd	1.94(2)	1(2)	-5(1)	0.0096	247.381	28.118	11

Zn-S(2.2) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(3)					
1Br	2.41(1)	4(1)					
1Br	2.66(3)	14(5)					
1Imd	2.07(1)	3(1)					
1Imd	1.94(1)	2(1)	-5(1)	0.0126	323.773	36.801	11

Zn-S(2.3) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	6(3)					
1Br	2.40(1)	4(1)					
1Br	2.66(3)	14(5)					
1Imd	2.07(1)	3(1)					
1Imd	1.94(1)	2(1)	-5(1)	0.0130	334.868	38.062	11

Zn-S(2.4) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.5) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(2)	3(4)					
1Br	2.40(1)	2(1)					
1Br	2.21(2)	2(4)					
1Imd	1.94(1)	1(2)					
1Imd	2.07(1)	2(2)	-5(1)	0.0093	238.180	27.072	11

Zn-S(2.6) Zn-Br(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.92(4)	5(6)					
1Br	2.36(3)	2(4)					
1Br	2.48(4)	5(7)					
1Imd	1.94(2)	3(2)					
1Imd	2.06(2)	4(2)	-5(2)	0.0355	912.310	103.697	11

Zn-S(2.2) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	6(2)					
1Br	2.41(1)	4(1)					
1Br	2.65(3)	13(5)					
1Imd	2.07(1)	3(1)					
1Imd	1.94(1)	2(1)	-5(1)	0.0124	317.724	36.114	11

Zn-S(2.3) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	6(3)					
1Br	2.41(1)	4(1)					
1Br	2.66(3)	13(5)					
1Imd	1.94(1)	2(1)					
1Imd	2.07(1)	3(1)	-5(1)	0.0128	327.743	37.253	11

Zn-S(2.4) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	6(3)					
1Br	2.41(1)	4(1)					
1Br	2.66(3)	13(5)					
1Imd	1.94(1)	2(1)					
1Imd	2.07(1)	3(1)	-5(1)	0.0131	336.450	38.242	11

Zn-S(2.5) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-S(2.6) Zn-Br(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.85(4)	6(4)					
1Br	2.39(1)	3(1)					
1Br	2.80(4)	2(4)					
1Imd	2.08(2)	5(2)					
1Imd	1.95(2)	5(2)	-4(2)	0.0452	1161.084	131.974	11

Table G.7. Additional Fits for Ni(II) E63C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	2(2)	5(5)	0.1975	950.791	139.886	3
3N/O	2.07(2)	4(1)	5(3)	0.0999	480.774	70.735	3
4N/O	2.07(1)	6(1)	4(2)	0.0681	328.113	48.274	3
5N/O	2.07(2)	8(1)	3(2)	0.0748	360.308	53.011	3
6N/O	2.06(2)	10(2)	2(2)	0.1027	494.249	72.717	3
7N/O	2.06(2)	12(2)	2(3)	0.1404	676.115	99.474	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.18(3)	6(2)	neg14(6)	0.1683	810.081	119.184	3
3S	2.18(2)	9(1)	neg14(4)	0.1097	528.176	77.709	3
4S	2.18(2)	12(1)	neg15(4)	0.0947	456.043	67.096	3
5S	2.18(2)	14(1)	neg15(4)	0.0995	478.850	70.452	3
6S	2.18(3)	16(2)	neg15(4)	0.1131	544.629	80.129	3
7S	2.18(3)	18(2)	neg16(4)	0.1305	628.443	92.461	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.02(2)	1(2)					
1N/O	2.15(2)	3(2)	4(2)	0.0576	277.295	57.807	5
2N/O	2.00(3)	3(4)					
2N/O	2.12(3)	2(3)	2(3)	0.0629	302.865	63.138	5
3N/O	2.03(2)	4(2)					
1N/O	2.15(3)	0(3)	3(2)	0.0586	282.277	58.846	5
4N/O	2.04(5)	10(5)	2(3)	0.0723	348.292	72.608	5

1N/O	2.09(6)	2(5)					
3N/O	2.08(4)	5(3)					
2N/O	2.00(0.10)	12(18)	1(3)	0.0679	327.160	68.203	5
5N/O	2.07(2)	8(2)					
1N/O	1.63(0.36)	53(92)	4(4)	0.0694	333.914	69.611	5
4N/O	2.06(2)	6(2)					
2N/O	1.95(9)	19(23)	0(3)	0.0699	336.371	70.123	5
3N/O	2.06(2)	5(2)					
3N/O	1.99(0.10)	19(17)	0(4)	0.0747	359.599	74.965	5
6N/O	2.08(2)	10(1)					
1N/O	2.45(3)	3(3)	4(2)	0.0444	213.908	44.593	5
5N/O	2.09(1)	8(1)					
2N/O	2.46(3)	10(5)	6(2)	0.0362	174.342	36.345	5
4N/O	2.09(2)	6(1)					
3N/O	2.43(6)	24(13)	7(2)	0.0541	260.580	54.323	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.14(4)	5(3)					
1S	2.26(5)	3(5)	neg14(6)	0.1009	486.019	101.320	5
2S	2.19(0.26)	16(14)					
2S	2.17(6)	9(5)	neg15(9)	0.0944	454.294	94.706	5
3S	2.18(3)	10(4)					
1S	2.29(0.30)	18(49)	neg13(8)	0.0922	444.141	92.590	5
4S	2.19(3)	11(2)					
1S	2.43(0.10)	14(16)	neg12(5)	0.0801	385.605	80.387	5
3S	2.18(3)	9(2)					
2S	2.34(0.13)	23(27)	neg11(6)	0.0817	393.131	81.956	5
5S	2.17(3)	14(2)					
1S	1.42(0.23)	39(56)	neg16(5)	0.0959	461.667	96.243	5
4S	2.20(3)	11(2)					
2S	2.43(7)	18(12)	neg10(4)	0.0691	332.617	69.340	5
3S	2.35(0.10)	25(22)					
3S	2.18(2)	9(2)	neg11(6)	0.0783	377.223	78.639	5

6S	2.18(4)	16(2)					
1S	1.02(0.11)	8(7)	neg16(6)	0.1204	579.778	120.866	5
5S	2.18(2)	14(1)					
2S	2.97(4)	11(5)	neg14(2)	0.0414	199.482	41.586	5
4S	2.20(2)	11(1)					
3S	2.44(5)	21(9)	neg9(4)	0.0597	287.635	59.963	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(4)	3(2)					5
1S	2.25(4)	4(3)	neg3(5)	0.0920	443.097	92.372	
1N/O	1.97(6)	3(4)					5
2S	2.22(4)	7(2)	neg9(6)	0.1077	518.441	108.079	
2N/O	2.00(7)	7(5)					
2S	2.22(4)	9(4)	neg7(7)	0.0963	463.479	96.621	5
3N/O	2.03(4)	7(3)					
1S	2.25(4)	7(5)	neg1(5)	0.0754	362.930	75.660	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.07(3)	8(4)					
1S	2.22(5)	11(11)	1(4)	0.0637	306.556	63.907	5
2N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.04(4)	7(5)					
2S	2.23(5)	13(8)	neg3(6)	0.0886	426.510	88.914	5
5N/O	2.09(4)	9(7)					
1S	2.19(9)	10(13)	3(3)	0.0542	260.982	54.407	5
1N/O	2.73(6)	2(6)					
5S	2.19(2)	14(1)	neg14(4)	0.0694	334.199	69.670	5
4N/O	2.07(2)	7(3)					
2S	2.21(5)	20(14)	0(4)	0.0764	367.967	76.710	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

3N/O	1.86(0.16)	24(21)					
3S	2.18(3)	9(2)	neg15(7)	0.0830	399.822	83.351	5
6N/O	2.11(3)	13(5)					
1S	2.20(4)	7(4)	3(3)	0.0545	262.640	54.752	5
1N/O	2.33(6)	2(6)					
6S	2.19(4)	16(3)	neg15(6)	0.0950	457.605	95.396	5
5N/O	2.08(3)	8(2)					
2S	2.17(6)	21(16)	1(3)	0.0647	311.746	64.989	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.06(2)	7(3)					
3S	2.21(6)	25(16)	neg2(5)	0.0845	406.700	84.784	5
3N/O	1.78(8)	22(16)					
4S	2.17(3)	11(2)	neg18(5)	0.0814	391.996	81.719	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.06(3)	2(2)					5
1Br	2.42(4)	11(4)	4(5)	0.1246	600.135	125.110	
1N/O	2.05(5)	1(3)					5
2Br	2.43(8)	14(6)	4(12)	0.2924	1407.835	293.490	
2N/O	2.07(3)	3(2)					
2Br	2.43(5)	17(5)	4(5)	0.1293	622.406	129.752	5
3N/O	2.06(2)	5(1)					
1Br	2.41(3)	12(4)	4(3)	0.0514	247.619	51.621	5
1N/O	2.06(5)	1(3)					
3Br	2.44(9)	18(6)	5(12)	0.2958	1424.053	296.871	5
1N/O	2.07(5)	1(3)					
4Br	2.45(9)	21(7)	5(12)	0.2985	1437.068	299.584	5
4N/O	2.07(1)	7(1)					
1Br	2.40(2)	13(3)	3(2)	0.0265	127.560	26.592	5
2N/O	2.07(3)	3(2)					
3Br	2.44(5)	21(6)	5(5)	0.1322	636.588	132.709	5
3N/O	2.07(2)	5(1)	4(3)	0.0535	257.727	53.728	5

2Br	2.42(3)	18(4)					
5N/O	2.07(1)	9(1)					
1Br	2.39(2)	13(3)	3(2)	0.0286	137.478	28.660	5
1N/O	2.07(5)	0(3)					
5Br	2.46(9)	23(7)	6(11)	0.3005	1446.998	301.654	5
4N/O	2.07(1)	7(1)					
2Br	2.40(2)	19(3)	4(2)	0.0257	123.535	25.753	5
2N/O	2.07(3)	3(2)					
4Br	2.44(6)	24(7)	5(5)	0.1343	646.799	134.838	5
3N/O	2.07(2)	5(1)					
3Br	2.42(4)	22(5)	4(2)	0.0549	264.098	55.056	5
6N/O	2.07(2)	12(2)					
1Br	2.38(3)	12(3)	2(2)	0.0449	216.348	45.102	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.08(1)	9(1)					
2Br	2.39(2)	18(3)	3(1)	0.0261	125.546	26.173	5
2N/O	2.07(3)	3(2)					
5Br	2.45(6)	26(7)	5(5)	0.1360	654.979	136.543	5
4N/O	2.08(1)	7(1)					
3Br	2.40(2)	23(4)	4(1)	0.0259	124.729	26.002	5
3N/O	2.08(2)	5(1)					
4Br	2.42(4)	25(5)	5(2)	0.0560	269.671	56.218	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.03(3)	2(2)					
1S	2.35(0.12)	6(12)					
1Br	2.35(0.10)	8(6)	1(5)	0.0601	289.303	103.438	7
1N/O	1.99(4)	0(4)					
2S	2.29(0.10)	7(7)					
1Br	2.30(0.11)	8(8)	neg4(7)	0.0775	373.085	133.394	7
1N/O	2.00(5)	2(4)					
1S	2.25(6)	1(4)					
2Br	2.26(0.18)	22(26)	neg4(8)	0.1199	577.192	206.370	7
3N/O	2.05(2)	5(2)	3(3)	0.0312	150.255	53.722	7

1S	2.43(0.12)	16(17)					
1Br	2.40(4)	10(4)					
2N/O	2.02(3)	3(2)					
2S	2.36(8)	15(9)					
1Br	2.37(5)	8(3)	0(4)	0.0472	227.101	81.198	7
2N/O	2.04(4)	2(3)					
1S	2.31(8)	4(5)					
2Br	2.32(0.10)	15(10)	0(5)	0.0574	276.287	98.784	7
1N/O	2.00(4)	0(3)					
2S	2.28(9)	6(5)					
2Br	2.29(0.11)	12(9)	neg4(7)	0.0683	328.861	117.582	7
4N/O	2.07(2)	7(1)					
1S	2.58(0.15)	25(31)					
1Br	2.42(5)	13(4)	4(2)	0.0208	99.934	35.730	7
3N/O	2.05(2)	5(1)					
2S	2.45(0.12)	29(16)					
1Br	2.41(4)	10(3)	2(3)	0.0271	130.689	46.727	7
3N/O	2.05(2)	5(2)					
1S	2.42(0.13)	11(15)					
2Br	2.40(6)	13(6)	3(3)	0.0275	132.274	47.293	7
2N/O	2.03(3)	4(2)					
2S	2.36(8)	12(8)					
2Br	2.36(6)	12(4)	0(4)	0.0381	183.635	65.657	7

Table G.8. Additional Fits for Ni(II) E63C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	3(1)	5(3)	0.2767	1569.419	79.911	3
3N/O	2.07(1)	5(1)	5(2)	0.1736	984.371	50.122	3
4N/O	2.07(1)	7(1)	4(2)	0.1366	774.591	39.440	3
5N/O	2.07(1)	8(1)	3(2)	0.1390	788.637	40.155	3
6N/O	2.07(1)	10(1)	3(2)	0.1638	928.805	47.292	3
7N/O	2.06(2)	12(1)	2(2)	0.1992	1130.114	57.542	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.18(2)	7(1)	14(4)	0.2341	1327.872	67.612	3
3S	2.18(2)	9(1)	neg14(3)	0.1742	988.060	50.309	3
4S	2.18(2)	12(1)	neg15(3)	0.1584	898.244	45.736	3

5S	2.18(2)	14(1)	neg15(3)	0.1624	921.150	46.903	3
6S	2.18(2)	16(1)	neg15(3)	0.1754	994.870	50.656	3
7S	2.18(2)	18(2)	neg16(3)	0.1922	1089.922	55.496	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.03(1)	0(1)					
1N/O	2.15(1)	2(1)	4(2)	0.1260	714.481	40.504	5
2N/O	2.00(2)	2(2)					
2N/O	2.12(2)	2(2)	3(2)	0.1252	710.284	40.266	5
3N/O	2.03(1)	4(1)					
1N/O	2.15(2)	0(2)	3(2)	0.1199	679.998	38.549	5
4N/O	2.04(3)	8(3)					
1N/O	2.12(5)	3(4)	2(2)	0.1392	789.368	44.750	5
3N/O	2.04(7)	10(7)					
2N/O	2.09(5)	5(3)	2(2)	0.1423	806.877	45.742	5
5N/O	2.05(4)	13(3)					
1N/O	2.08(4)	3(3)	2(2)	0.1597	905.617	51.340	5
4N/O	2.06(1)	7(1)					
2N/O	1.97(0.10)	24(26)	1(3)	0.1401	794.854	45.061	5
3N/O	2.07(2)	5(1)					
3N/O	2.01(8)	20(13)	0(3)	0.1475	836.350	47.413	5
6N/O	2.08(1)	10(1)					
1N/O	2.45(2)	3(3)	4(2)	0.1085	615.522	34.894	5
5N/O	2.07(2)	8(1)					
2N/O	1.62(0.18)	68(54)	4(3)	0.1317	746.940	42.344	5
4N/O	2.09(1)	6(1)					
3N/O	2.43(5)	24(11)	8(2)	0.1243	705.259	39.981	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.13(2)	6(2)					
1S	2.26(3)	3(2)	neg15(4)	0.1622	919.881	52.148	5
2S	2.16(7)	9(5)					
2S	2.22(0.15)	14(13)	neg14(5)	0.1578	895.177	50.748	5
3S	2.17(3)	10(3)					
1S	2.27(0.26)	18(34)	neg13(6)	0.1572	891.378	50.533	5

4S	2.19(2)	11(1)					
1S	2.43(7)	14(12)	neg12(4)	0.1453	824.373	46.734	5
3S	2.18(2)	9(2)					
2S	2.34(0.10)	24(21)	neg11(5)	0.1478	838.115	47.513	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.20(2)	11(1)					
2S	2.43(5)	18(9)	neg10(3)	0.1350	765.812	43.414	5
3S	2.19(2)	9(1)					
3S	2.37(7)	26(14)	neg10(4)	0.1390	788.564	44.704	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.21(2)	12(1)					
2S	2.47(3)	14(5)	neg9(3)	0.1251	709.687	40.232	5
4S	2.20(2)	11(1)					
3S	2.44(4)	21(7)	neg9(3)	0.1260	714.592	40.511	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(2)	4(1)					5
1S	2.25(2)	4(2)	neg3(3)	0.1525	864.947	49.034	
1N/O	1.97(3)	3(2)					5
2S	2.22(2)	7(1)	neg9(4)	0.1669	946.588	53.663	
2N/O	2.00(4)	7(3)					
2S	2.23(3)	9(2)	neg7(4)	0.1568	889.072	50.402	5
3N/O	2.03(3)	7(2)					
1S	2.25(3)	7(3)	neg2(3)	0.1373	778.912	44.157	5
1N/O	2.71(7)	6(8)					
3S	2.19(2)	9(1)	neg12(3)	0.1593	903.377	51.213	5
1N/O	2.71(5)	5(6)					
4S	2.19(2)	12(1)	neg13(3)	0.1386	785.914	44.554	5
4N/O	2.06(3)	9(3)					
1S	2.23(3)	10(6)	1(3)	0.1296	734.843	41.659	5
2N/O	1.87(0.13)	21(15)	neg15(5)	0.1526	865.312	49.055	5

3S	2.18(2)	9(1)					
3N/O	2.04(3)	9(4)					
2S	2.23(3)	12(4)	neg4(4)	0.1513	858.035	48.642	5
5N/O	2.09(3)	9(5)					
1S	2.19(6)	10(9)	3(3)	0.1221	692.297	39.247	5
1N/O	2.34(7)	5(6)					
5S	2.19(3)	14(2)	neg16(4)	0.1578	895.115	50.745	5
4N/O	2.06(2)	8(3)					
2S	2.22(3)	17(8)	neg1(3)	0.1430	811.269	45.991	5
2N/O	2.73(5)	8(6)					
4S	2.19(2)	12(1)	neg12(2)	0.1287	730.238	41.398	5
3N/O	1.88(0.14)	26(16)					
3S	2.18(2)	9(1)	neg15(5)	0.1503	852.439	48.325	5
6N/O	2.11(3)	12(4)					
1S	2.20(4)	7(3)	3(3)	0.1231	697.947	39.567	5
1N/O	2.34(5)	3(4)					
6S	2.19(3)	17(2)	neg15(4)	0.1597	906.047	51.364	5
5N/O	2.08(2)	8(2)					
2S	2.18(4)	20(11)	1(3)	0.1333	756.184	42.868	5
2N/O	2.73(4)	7(5)					
5S	2.19(2)	14(1)	neg13(2)	0.1276	723.957	41.041	5
4N/O	2.06(2)	8(2)					
3S	2.21(4)	22(9)	neg2(4)	0.1510	856.556	48.559	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.06(2)	3(1)					5
1Br	2.41(3)	11(3)	4(3)	0.2024	1147.806	65.070	
1N/O	2.05(3)	1(2)					5
2Br	2.42(5)	14(3)	3(7)	0.3701	2098.925	118.989	
2N/O	2.06(2)	3(1)					
2Br	2.43(3)	16(3)	4(3)	0.2027	1149.853	65.186	5

3N/O	2.06(1)	5(1)					
1Br	2.41(2)	12(3)	4(2)	0.1222	693.351	39.306	5
1N/O	2.06(3)	1(2)					
3Br	2.43(5)	18(4)	4(7)	0.3700	2098.815	118.983	5
1N/O	2.06(3)	1(2)					
4Br	2.44(5)	20(4)	4(7)	0.3715	2106.858	119.439	5
4N/O	2.07(1)	7(1)					
1Br	2.40(2)	13(3)	3(2)	0.0936	530.966	30.101	5
2N/O	2.07(2)	3(1)					
3Br	2.43(3)	20(4)	4(3)	0.2043	1158.646	65.684	5
3N/O	2.07(1)	5(1)					
2Br	2.42(3)	18(3)	4(2)	0.1229	697.215	39.525	5
5N/O	2.07(1)	10(1)					
1Br	2.39(2)	14(3)	3(2)	0.0937	531.602	30.137	5
1N/O	2.07(3)	1(2)					
5Br	2.45(5)	23(4)	5(6)	0.3733	2117.099	120.019	5
4N/O	2.07(1)	7(1)					
2Br	2.40(2)	19(3)	4(2)	0.0926	525.245	29.776	5
2N/O	2.07(2)	3(1)					
4Br	2.44(4)	23(4)	5(3)	0.2061	1169.229	66.284	5
3N/O	2.07(1)	5(1)					
3Br	2.42(3)	22(4)	4(2)	0.1241	703.844	39.901	5
6N/O	2.07(2)	12(1)					
1Br	2.38(2)	12(3)	2(2)	0.1090	618.064	35.038	5
1N/O	1.69(3)	5(3)					
6Br	2.20(3)	15(1)	neg46(6)	0.2380	1350.120	76.539	5
5N/O	2.08(1)	10(1)					
2Br	2.39(2)	18(3)	3(1)	0.0912	517.412	29.332	5
2N/O	2.07(2)	3(1)					
5Br	2.44(4)	25(4)	5(3)	0.2082	1180.780	66.939	5
4N/O	2.08(1)	7(1)					
3Br	2.41(2)	22(3)	4(2)	0.0930	527.219	29.888	5
3N/O	2.08(1)	5(1)					
4Br	2.43(3)	25(4)	4(2)	0.1256	712.274	40.379	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(2)	3(1)					
1S	2.32(7)	6(6)					
1Br	2.34(7)	10(5)	0(3)	0.1326	752.307	48.103	7
1N/O	1.99(2)	1(2)					
2S	2.27(6)	7(4)					
1Br	2.29(8)	10(6)	neg5(4)	0.1445	819.747	52.415	7
1N/O	2.00(2)	0(2)					
1S	2.24(3)	3(2)					
2Br	2.30(0.14)	29(24)	neg5(5)	0.1959	1110.884	71.030	7
3N/O	2.05(2)	6(1)					
1S	2.39(8)	14(11)					
1Br	2.38(4)	10(3)	2(2)	0.1014	575.242	36.781	7
2N/O	2.02(2)	4(2)					
2S	2.33(5)	13(5)					
1Br	2.35(3)	9(2)	neg1(3)	0.1149	651.755	41.673	7
2N/O	2.03(2)	3(2)					
1S	2.28(4)	4(2)					
2Br	2.30(6)	19(9)	neg1(3)	0.1297	735.425	47.023	7
1N/O	2.00(2)	1(2)					
2S	2.27(5)	6(3)					
2Br	2.27(7)	15(7)	neg5(4)	0.1395	791.158	50.587	7
4N/O	2.07(2)	7(1)					
1S	2.59(0.14)	27(29)					
1Br	2.41(4)	13(4)	4(2)	0.0876	496.633	31.755	7
3N/O	2.05(2)	6(1)					
2S	2.41(9)	27(11)					
1Br	2.39(3)	10(2)	2(2)	0.0972	551.291	35.250	7
3N/O	2.05(2)	6(1)					
1S	2.40(0.10)	12(12)					
2Br	2.39(5)	14(4)	2(2)	0.0971	550.813	35.219	7
2N/O	2.02(2)	4(2)					
2S	2.34(6)	11(5)					
2Br	2.35(4)	12(3)	neg1(3)	0.1061	601.646	38.469	7

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(2)	13(2)	3(2)	0.1060	792.027	53.523	5

1Imd	2.06(2)	3(3)					
4N/O	2.07(2)	9(3)					
1Imd	2.06(4)	4(5)					
1Imd	1.93(7)	11(13)	1(2)	0.0851	443.637	34.665	7
3N/O	2.07(2)	6(2)					
1Imd	1.97(2)	4(2)					
1Imd	1.84(2)	1(3)					
1Imd	2.11(2)	3(2)	0(1)	0.0506	263.889	24.439	9
2N/O	2.08(2)	4(2)					
1Imd	1.84(0.12)	17(21)					
1Imd	2.01(2)	1(2)					
1Imd	1.51(5)	13(5)					
1Imd	2.15(2)	1(2)	5(3)	0.0406	211.472	24.037	11
1N/O	2.07(2)	1(2)					
1Imd	2.05(2)	14(3)					
1Imd	1.60(0.19)	26(26)					
1Imd	1.93(3)	11(3)					
1Imd	2.17(2)	10(2)					
1Imd	1.82(3)	5(5)	1(2)	0.0473	246.416	36.249	13
4N/O	2.07(2)	9(2)					
1Imd	2.05(4)	5(4)	3(2)	0.0892	464.671	31.401	5
3N/O	2.07(2)	6(2)					
1Imd	1.97(5)	6(7)					
1Imd	2.09(5)	4(7)	2(2)	0.0727	378.797	29.598	7
2N/O	2.07(2)	3(2)					
1Imd	1.99(2)	4(2)					
1Imd	2.12(2)	4(2)					
1Imd	1.87(3)	1(3)	0(1)	0.0477	248.437	23.008	9
1N/O	2.07(2)	1(2)					
1Imd	2.17(2)	9(2)					
1Imd	1.83(2)	5(3)					
1Imd	2.05(2)	12(2)					
1Imd	1.93(2)	11(2)	0(1)	0.0518	270.058	30.696	11
0N/O							
1Imd	1.97(3)	13(4)					
1Imd	2.19(3)	10(4)					
1Imd	1.86(3)	6(5)					
1Imd	2.08(3)	14(4)					
1Imd	2.29(0.41)	31(135)	1(3)	0.1432	745.893	84.781	11
3N/O	2.08(2)	6(2)	4(2)	0.0880	458.528	30.986	5

1Imd	2.04(4)	5(4)					
2N/O	2.07(2)	3(2)					
1Imd	2.13(3)	1(2)					
1Imd	1.98(2)	0(2)	4(1)	0.0700	364.857	28.509	7
1N/O	2.06(2)	1(2)					
1Imd	2.01(2)	5(3)					
1Imd	2.15(2)	4(2)					
1Imd	1.91(3)	0(4)	1(2)	0.0693	361.310	33.461	9
0N/O							
1Imd	1.86(3)	6(4)					
1Imd	2.08(3)	13(3)					
1Imd	2.19(3)	10(3)					
1Imd	1.97(2)	13(3)	1(2)	0.1445	752.725	69.711	9
2N/O	2.08(2)	4(3)					
1Imd	2.04(5)	4(4)	4(2)	0.1256	654.141	44.205	5
1N/O	2.07(2)	0(2)					
1Imd	2.14(2)	2(2)					
1Imd	1.99(2)	2(1)	4(2)	0.1019	531.145	41.503	7
0N/O							
1Imd	2.15(3)	6(3)					
1Imd	1.94(4)	2(7)					
1Imd	2.03(3)	6(4)	2(2)	0.1806	940.923	73.522	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(3)	8(5)					
1S	2.23(3)	9(7)					
1Imd	2.01(4)	4(3)	1(3)	0.0805	419.524	32.781	7
2N/O	2.05(4)	5(3)					
1S	2.25(2)	6(3)					
1Imd	1.86(6)	7(6)					
1Imd	1.99(4)	2(3)	neg4(3)	0.0648	337.501	31.256	9
1N/O	2.04(3)	0(3)					
1S	2.27(3)	7(4)					
1Imd	1.95(3)	5(2)					
1Imd	2.08(3)	4(3)					
1Imd	1.82(3)	0(3)	neg4(2)	0.0514	267.874	30.448	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(3)	7(4)					
1S	2.23(3)	11(8)	1(3)	0.084	437.403	34.178	7

1Imd	2.00(4)	4(3)					
2N/O	2.05(4)	5(3)					
1S	2.25(2)	6(3)					
1Imd	1.99(4)	2(3)					
1Imd	1.86(6)	7(6)	neg4(3)	0.0677	352.800	32.673	9
1N/O	2.04(3)	0(3)					
1S	2.28(3)	8(4)					
1Imd	1.95(3)	5(2)					
1Imd	2.08(3)	4(3)					
1Imd	1.82(3)	0(3)	neg4(2)	0.0544	283.258	32.196	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	6(2)					
1S	2.67(3)	11(4)					
1Imd	2.07(3)	5(4)	5(1)	0.0574	299.253	23.383	7
2N/O	2.05(4)	5(3)					
1S	2.25(2)	6(3)					
1Imd	1.99(4)	2(3)					
1Imd	1.86(6)	7(6)	neg4(3)	0.0702	365.690	33.867	9
1N/O	2.04(3)	0(3)					
1S	2.28(3)	8(4)					
1Imd	2.08(3)	4(3)					
1Imd	1.95(3)	5(2)					
1Imd	1.82(4)	0(3)	neg4(2)	0.0567	295.605	33.600	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	6(2)					
1S	2.67(3)	11(4)					
1Imd	2.07(3)	5(4)	5(1)	0.0585	304.652	23.805	7
2N/O	2.07(2)	4(2)					
1S	2.66(3)	11(4)					
1Imd	2.15(2)	0(2)					
1Imd	2.00(2)	0(2)	5(1)	0.0471	245.355	22.723	9
1N/O							
1S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

3N/O	2.07(2)	6(2)					
1S	2.67(3)	11(4)					
1Imd	2.07(3)	5(4)	5(1)	0.0595	310.095	24.230	7
2N/O	2.07(2)	4(2)					
1S	2.66(3)	12(4)					
1Imd	2.15(2)	0(2)					
1Imd	2.00(2)	0(2)	4(1)	0.0485	252.847	23.416	9
1N/O	2.06(2)	0(2)					
1S	2.62(9)	22(16)					
1Imd	2.15(2)	4(2)					
1Imd	2.02(3)	4(3)					
1Imd	1.92(4)	0(6)	2(2)	0.0653	340.282	38.678	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	3(3)					
2S	2.24(4)	16(5)					
1Imd	1.97(4)	4(4)	neg2(3)	0.1008	525.393	41.053	7
1N/O	2.04(5)	2(4)					
2S	2.24(2)	9(2)					
1Imd	1.97(4)	2(3)					
1Imd	1.83(5)	7(6)	neg7(3)	0.0834	434.643	40.253	9
0N/O							
2S	2.25(2)	9(3)					
1Imd	1.93(4)	5(3)					
1Imd	2.06(4)	4(3)					
1Imd	1.80(4)	0(4)	neg6(3)	0.0993	517.321	47.910	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	3(2)					
2S	2.25(4)	16(6)					
1Imd	1.96(4)	4(4)	neg3(3)	0.1066	555.410	43.399	7
1N/O	2.04(5)	2(4)					
2S	2.24(2)	9(2)					
1Imd	1.96(4)	2(3)					
1Imd	1.82(5)	6(6)	neg7(3)	0.0886	461.724	42.761	9
0N/O							
2S	2.25(2)	9(3)					
1Imd	2.06(4)	5(3)					
1Imd	1.93(4)	5(3)					
1Imd	1.80(4)	0(4)	neg7(3)	0.1073	558.987	51.768	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	3(2)					
2S	2.25(4)	17(6)					
1Imd	1.96(4)	4(4)	neg3(3)	0.1112	579.622	45.291	7
1N/O	2.04(4)	1(4)					
2S	2.24(2)	9(3)					
1Imd	1.96(4)	2(3)					
1Imd	1.82(5)	6(6)	neg8(3)	0.0928	483.320	44.761	9
0N/O							
2S	2.25(3)	10(3)					
1Imd	2.06(4)	5(3)					
1Imd	1.93(4)	5(3)					
1Imd	1.80(4)	0(4)	neg7(3)	0.1135	591.577	54.787	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	4(3)					
2S	2.69(7)	28(12)					
1Imd	2.07(5)	5(5)	6(2)	0.1112	579.587	45.288	7
1N/O	2.07(2)	0(2)					
2S	2.63(0.14)	43(27)					
1Imd	1.99(2)	2(1)					
1Imd	2.14(2)	2(2)	5(2)	0.0922	480.294	44.481	9
0N/O							
2S	2.25(3)	10(3)					
1Imd	1.93(4)	5(3)					
1Imd	1.80(4)	0(4)					
1Imd	2.05(4)	5(3)	neg7(3)	0.1186	618.086	57.242	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	4(3)					
2S	2.69(8)	30(14)					
1Imd	2.07(5)	5(5)	5(2)	0.1122	584.826	45.697	7
1N/O	2.07(2)	0(2)					
2S	2.63(0.15)	45(29)					
1Imd	1.99(2)	2(1)					
1Imd	2.14(2)	2(2)	4(2)	0.0932	485.408	44.954	9
0N/O							
2S	2.25(3)	10(3)					
1Imd	2.05(4)	5(3)					
1Imd	1.93(4)	5(3)					
1Imd	1.79(4)	0(4)	neg8(3)	0.1226	638.748	59.155	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.57(3)	9(4)					
1S	2.30(3)	7(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0533	277.762	25.724	9
1N/O	2.04(2)	1(2)					
1S	2.30(3)	4(3)					
1S	2.55(4)	8(4)					
1Imd	1.94(4)	2(3)					
1Imd	2.08(4)	2(4)	0(2)	0.0371	193.475	21.991	11
1N/O	2.04(3)	0(3)					
1S	2.30(3)	5(3)					
1S	2.55(4)	9(4)					
1Imd 0°	2.07(4)	2(5)					
1Imd 5°	1.94(5)	2(4)	0(2)	0.0404	301.825	34.307	11
1N/O	2.01(3)	2(4)					
1S	2.55(4)	8(4)					
1S	2.30(3)	6(3)					
1Imd 0°	2.00(5)	6(5)					
1Imd 10°	2.08(4)	3(4)	1(2)	0.0414	215.883	24.538	11
1N/O	2.01(4)	2(4)					
1S	2.56(4)	8(4)					
1S	2.30(3)	6(3)					
1Imd 5°	2.02(5)	6(5)					
1Imd 10°	2.09(4)	2(4)	1(2)	0.044	229.261	26.059	11
0N/O							
1S	2.25(2)	4(3)					
1S	2.46(8)	15(11)					
1Imd	2.10(5)	2(6)					
1Imd	1.98(4)	3(5)					
1Imd	1.88(6)	2(7)	neg2(3)	0.0735	382.869	43.518	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.29(2)	7(2)					
1S	2.58(3)	10(4)					
1Imd	2.02(3)	4(3)	1(2)	0.0491	256.072	23.715	9
1N/O	2.03(2)	0(2)					
1S	2.29(2)	4(3)					
1S	2.55(4)	9(4)					
1Imd	1.94(4)	2(3)	0(2)	0.0368	191.937	21.816	11

1Imd	2.07(4)	2(4)					
1N/O	2.04(3)	0(3)					
1S	2.29(2)	4(3)					
1S	2.55(4)	10(5)					
1Imd 0°	2.05(5)	3(6)					
1Imd 5°	1.94(5)	3(5)	0(2)	0.0399	207.873	23.628	11
1N/O	2.01(3)	2(4)					
1S	2.29(2)	6(2)					
1S	2.56(4)	10(4)					
1Imd 0°	2.00(5)	6(5)					
1Imd 10°	2.09(4)	3(4)	1(2)	0.0394	205.247	23.329	11
1N/O	2.01(4)	2(4)					
1S	2.29(3)	6(3)					
1S	2.56(4)	10(5)					
1Imd 5°	2.02(5)	6(5)					
1Imd 10°	2.09(4)	3(4)	1(2)	0.0423	220.399	25.051	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.29(2)	7(2)					
1S	2.58(3)	11(4)					
1Imd	2.02(3)	4(3)	1(2)	0.0484	252.130	23.350	9
1N/O	2.03(2)	0(2)					
1S	2.29(2)	4(2)					
1S	2.55(4)	10(4)					
1Imd	1.94(4)	3(4)					
1Imd	2.07(4)	3(4)	neg1(2)	0.0363	189.175	21.502	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	6(3)					
1S	2.29(2)	7(2)					
1S	2.58(3)	11(4)					
1Imd	2.02(3)	4(3)	1(2)	0.0479	249.359	23.093	9
1N/O	2.03(2)	0(2)					
1S	2.29(2)	4(2)					
1S	2.55(4)	10(4)					
1Imd	2.06(4)	3(5)					
1Imd	1.93(5)	3(4)	neg1(2)	0.0358	186.680	21.219	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.57(3)	9(4)	1(2)	0.054	281.102	26.033	9

1S	2.30(3)	7(3)					
1Imd	2.01(4)	4(4)					
1N/O	2.04(2)	1(2)					
1S	2.30(3)	5(3)					
1S	2.56(4)	8(4)					
1Imd	2.08(4)	2(4)					
1Imd	1.94(4)	2(3)	0(2)	0.0378	197.184	22.413	11
1N/O	2.04(3)	0(3)					
1S	2.30(3)	5(3)					
1S	2.55(4)	9(4)					
1Imd 0°	2.06(4)	3(5)					
1Imd 5°	1.94(5)	3(4)	0(2)	0.0412	214.650	24.398	11
1N/O	2.01(4)	2(4)					
1S	2.55(4)	9(4)					
1S	2.30(3)	6(3)					
1Imd 0°	2.00(5)	6(5)					
1Imd 10°	2.08(4)	3(4)	0(2)	0.0423	220.344	25.045	11
1N/O	2.01(4)	2(5)					
1S	2.56(4)	8(4)					
1S	2.30(3)	6(3)					
1Imd 5°	2.01(5)	5(5)					
1Imd 10°	2.09(4)	2(4)	1(2)	0.045	234.692	26.676	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.29(3)	7(2)					
1S	2.58(3)	10(4)					
1Imd	2.02(3)	4(3)	1(2)	0.0503	262.181	24.281	9
1N/O	2.04(2)	1(2)					
1S	2.29(2)	4(3)					
1S	2.55(4)	9(4)					
1Imd	2.07(4)	2(4)					
1Imd	1.94(4)	2(3)	0(2)	0.0373	194.535	22.112	11
1N/O	2.04(3)	0(3)					
1S	2.29(2)	4(3)					
1S	2.55(4)	10(4)					
1Imd 0°	2.05(5)	3(6)					
1Imd 5°	1.94(5)	3(6)	neg1(2)	0.0405	211.063	23.990	11
1N/O	2.01(4)	2(4)					
1S	2.29(2)	6(3)					
1S	2.56(4)	10(4)					
1Imd 0°	1.99(5)	6(5)	0(2)	0.0405	210.825	23.963	11

1Imd 10°	2.09(4)	3(4)					
1N/O	2.01(4)	3(5)					
1S	2.29(3)	6(3)					
1S	2.56(4)	10(4)					
1Imd 5°	2.01(5)	5(5)					
1Imd 10°	2.09(4)	3(4)	1(2)	0.0435	226.754	25.774	11
0N/O							
1S	2.25(3)	4(3)					
1S	2.48(7)	15(10)					
1Imd	2.10(5)	2(6)					
1Imd	1.88(6)	2(8)					
1Imd	1.98(4)	3(5)	neg2(3)	0.0744	387.723	44.070	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.29(2)	7(2)					
1S	2.58(3)	10(4)					
1Imd	2.02(3)	4(3)	1(2)	0.0497	259.138	23.999	9
1N/O	2.03(2)	0(2)					
1S	2.29(2)	4(2)					
1S	2.55(4)	9(4)					
1Imd	2.07(4)	3(4)					
1Imd	1.93(4)	3(4)	neg1(2)	0.0369	192.054	21.830	11
1N/O	2.04(3)	0(3)					
1S	2.29(2)	4(2)					
1S	2.55(4)	10(5)					
1Imd 0°	2.04(5)	3(6)					
1Imd 5°	1.93(6)	4(7)	neg1(2)	0.0399	207.938	23.635	11
1N/O	2.01(4)	2(4)					
1S	2.29(2)	6(2)					
1S	2.56(4)	10(4)					
1Imd 0°	1.99(5)	6(5)					
1Imd 10°	2.09(4)	3(4)	0(2)	0.0402	209.503	23.813	11
1N/O	2.01(4)	3(5)					
1S	2.29(3)	6(3)					
1S	2.57(4)	10(5)					
1Imd 5°	2.01(5)	5(5)					
1Imd 10°	2.09(4)	3(4)	1(2)	0.0434	226.019	25.690	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.57(4)	9(4)	1(2)	0.0549	285.961	26.483	9

1S	2.30(3)	7(3)					
1Imd	2.01(4)	4(4)					
1N/O	2.04(2)	1(2)					
1S	2.30(2)	5(3)					
1S	2.56(4)	8(4)					
1Imd	2.07(4)	2(4)					
1Imd	1.94(4)	2(3)	0(2)	0.0384	199.960	22.728	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.29(3)	7(2)					
1S	2.58(3)	10(4)					
1Imd	2.01(3)	4(3)	1(2)	0.0515	268.219	24.840	9
1N/O	2.04(2)	0(2)					
1S	2.30(2)	4(3)					
1S	2.55(4)	9(4)					
1Imd	2.07(4)	2(4)					
1Imd	1.93(4)	2(3)	neg1(2)	0.0379	197.376	22.435	11

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.58(4)	9(4)					
1S	2.30(3)	7(3)					
1Imd	2.01(4)	4(4)	0(2)	0.0554	288.440	26.713	9
1N/O	2.04(2)	1(2)					
1S	2.56(4)	7(3)					
1S	2.30(3)	5(3)					
1Imd	2.07(4)	2(4)					
1Imd	1.94(3)	1(3)	neg1(2)	0.0407	211.816	24.076	11
0N/O							
1S	2.26(3)	5(3)					
1S	2.49(7)	14(9)					
1Imd	2.88(6)	2(8)					
1Imd	1.98(4)	4(5)					
1Imd	2.10(5)	3(6)	neg2(3)	0.0788	410.498	46.659	11

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.39(7)	10(8)					
1Br	2.38(4)	9(3)					
1Imd	2.03(4)	4(4)	2(2)	0.0533	277.498	25.699	9

1N/O	2.04(2)	0(2)					
1S	2.38(5)	5(7)					
1Br	2.36(4)	7(4)					
1Imd	2.09(4)	2(3)					
1Imd	1.95(3)	1(3)	1(2)	0.0407	212.124	24.111	11

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.38(7)	11(8)					
1Br	2.38(4)	9(3)					
1Imd	2.03(4)	4(4)	1(2)	0.0528	275.314	25.497	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.38(7)	11(8)					
1Br	2.38(4)	9(3)					
1Imd	2.03(4)	4(4)	1(2)	0.0526	274.151	25.389	9
1N/O	2.04(2)	0(2)					
1S	2.37(5)	5(7)					
1Br	2.36(5)	8(3)					
1Imd	2.09(4)	2(3)					
1Imd	1.95(3)	1(3)	1(2)	0.0402	209.394	23.801	11

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(4)	7(5)					
1S	2.26(3)	7(3)					
1Br	2.77(6)	15(7)					
1Imd	2.01(4)	4(4)	neg1(3)	0.0794	413.759	38.319	9
1N/O	2.04(5)	1(4)					
1S	2.27(2)	5(3)					
1Br	2.74(6)	16(8)					
1Imd	1.92(0.12)	7(15)					
1Imd	2.01(8)	3(7)	neg3(3)	0.0651	339.332	38.570	11

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.40(6)	11(9)	1(2)	0.0538	280.552	25.982	9

1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)					
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.39(6)	11(8)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0535	278.495	25.792	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.39(6)	11(8)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0533	277.480	25.698	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(4)	6(4)					
1S	2.27(3)	8(3)					
1Br	2.77(6)	16(7)					
1Imd	2.00(5)	4(4)	neg1(3)	0.084	437.760	40.541	9
1N/O	2.04(5)	1(4)					
1S	2.27(3)	6(4)					
1Br	2.73(6)	15(8)					
1Imd	1.93(0.13)	7(17)					
1Imd	2.01(9)	3(7)	neg3(3)	0.0689	359.059	40.812	11

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(2)	5(3)					
1S	2.41(6)	11(9)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0543	283.157	26.223	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.40(6)	11(9)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.054	281.232	26.045	9
1N/O	2.04(2)	1(2)					
1S	2.39(5)	5(7)					
1Br	2.37(4)	6(4)					
1Imd	2.09(4)	2(3)					
1Imd	1.95(3)	1(3)	0(2)	0.0402	209.581	23.822	11

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.39(6)	11(8)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0538	280.339	25.963	9
1N/O	2.04(2)	0(2)					
1S	2.38(5)	5(7)					
1Br	2.37(4)	7(3)					
1Imd	1.95(3)	1(3)					
1Imd	2.09(4)	2(3)	0(2)	0.0402	209.292	23.789	11

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.05(5)	1(4)					
1S	2.27(3)	6(4)					
1Br	2.73(6)	15(8)					
1Imd	1.93(0.14)	7(18)	neg3(4)	0.072	375.121	42.638	11

1Imd	2.01(0.10)	3(7)					

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(2)	5(3)					
1S	2.41(6)	12(9)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	5(4)	1(2)	0.055	286.350	26.519	9
1N/O	2.04(2)	1(2)					
1S	2.40(5)	5(7)					
1Br	2.37(4)	6(4)					
1Imd	2.08(4)	2(3)					
1Imd	1.94(3)	1(3)	0(2)	0.0406	211.683	24.061	11

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(2)	5(3)					
1S	2.40(6)	12(9)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0546	284.579	26.355	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.40(6)	12(9)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0545	283.798	26.283	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.39(6)	12(8)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	4(4)	1(2)	0.0543	282.749	26.186	9
1N/O	2.07(3)	0(3)	5(2)	0.0844	439.971	50.009	11

1S	2.66(8)	11(9)					
1Br	2.68(0.88)	39(158)					
1Imd	2.15(2)	2(2)					
1Imd	2.00(2)	2(2)					

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(2)	5(3)					
1S	2.42(6)	12(9)					
1Br	2.38(3)	9(3)					
1Imd	2.02(4)	5(4)	1(2)	0.0555	289.323	26.795	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(2)	5(3)					
1S	2.41(6)	12(9)					
1Br	2.39(3)	9(3)					
1Imd	2.02(4)	5(4)	1(2)	0.0552	287.717	26.646	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.40(6)	12(9)					
1Br	2.39(3)	9(3)					
1Imd	2.02(4)	5(4)	1(2)	0.0551	287.059	26.585	9
1N/O							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	5(3)					
1S	2.40(6)	12(9)					
1Br	2.39(3)	9(3)	1(2)	0.0549	286.137	26.499	9

1Imd	2.02(4)	5(4)					
1N/O	2.04(2)	0(2)					
1S	2.39(5)	6(7)					
1Br	2.37(4)	7(3)					
1Imd	2.0894)	2(3)					
1Imd	1.94(3)	1(3)	0(2)	0.0407	212.172	24.116	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.27(3)	6(4)					
1S	2.46(5)	2(5)					
1Br	2.41(5)	2(5)					
1Imd	2.01(4)	3(4)	0(2)	0.0544	283.305	32.202	11
0N/O							
1S	2.24(2)	3(4)					
1S	2.37(4)	2(5)					
1Br	2.32(5)	3(5)					
1Imd	1.95(0.18)	9(20)					
1Imd	1.99(0.10)	3(5)	neg4(3)	0.0579	301.690	34.291	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.27(3)	5(3)					
1S	2.47(5)	2(5)					
1Br	2.41(5)	2(5)					
1Imd	2.01(4)	3(4)	0(2)	0.0525	273.720	31.112	11
0N/O							
1S	2.24(2)	3(3)					
1S	2.37(4)	1(4)					
1Br	2.33(5)	4(5)					
1Imd	1.95(0.17)	9(19)					
1Imd	1.99(9)	3(5)	neg3(3)	0.0565	294.387	33.461	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(4)	3(3)					
1S	2.27(5)	0(3)					
1S	3.14(0.10)	13(13)					
1Br	2.24(0.10)	11(8)					
1Imd	1.94(6)	4(5)	neg4(4)	0.0636	331.369	37.665	11
0N/O							
1S	2.23(2)	2(3)					
1S	2.37(4)	1(4)	neg3(3)	0.0554	288.719	32.817	11

1Br	2.33(5)	4(5)					
1Imd	1.99(9)	3(5)					
1Imd	1.95(0.16)	9(18)					

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(4)	1(4)					
1S	2.49(6)	6(6)					
1S	2.28(3)	2(2)					
1Br	2.81(5)	10(5)					
1Imd	2.04(5)	1(4)	0(3)	0.0677	352.978	40.121	11
0N/O							
1S	2.24(3)	2(3)					
1S	2.40(6)	9(8)					
1Br	2.75(4)	10(4)					
1Imd	2.01(5)	0(3)					
1Imd	1.95(0.10)	7(13)	neg3(3)	0.0702	365.895	41.589	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	0(4)					
1S	2.25(4)	7(5)					
1S	2.46(5)	3(4)					
1Br	2.41(5)	1(5)					
1Imd	2.00(4)	3(4)	neg1(2)	0.052	270.899	30.792	11
0N/O							
1S	2.23(2)	4(3)					
1S	2.39(4)	2(5)					
1Br	2.34(5)	2(6)					
1Imd	1.98(6)	2(3)					
1Imd	1.94(0.14)	11(18)	neg4(3)	0.0563	293.243	33.331	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.26(3)	6(4)					
1S	2.47(5)	3(4)					
1Br	2.41(4)	1(4)					
1Imd	2.01(4)	3(4)	0(2)	0.0504	262.397	29.825	11
0N/O							
1S	2.23(2)	3(3)					
1S	2.39(4)	2(5)					
1Br	2.34(4)	3(5)					
1Imd	1.99(6)	2(3)					
1Imd	1.95(0.13)	11(17)	neg4(3)	0.0546	284.381	32.324	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	2(4)					
1S	2.26(3)	5(3)					
1S	2.47(5)	2(4)					
1Br	2.42(4)	2(5)					
1Imd	2.01(4)	3(4)	0(2)	0.0497	258.780	29.414	11
0N/O							
1S	2.23(2)	3(3)					
1S	2.39(4)	2(5)					
1Br	2.34(4)	3(5)					
1Imd	1.95(0.13)	10(17)					
1Imd	1.99(6)	2(3)	neg4(2)	0.0535	278.586	31.665	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	2(4)					
1S	2.26(3)	5(3)					
1S	2.47(5)	2(4)					
1Br	2.42(4)	2(5)					
1Imd	2.01(4)	2(4)	0(2)	0.049	255.287	29.017	11
0N/O							
1S	2.23(2)	3(3)					
1S	2.39(4)	1(4)					
1Br	2.34(4)	3(5)					
1Imd	1.95(0.13)	10(16)					
1Imd	1.99(6)	2(3)	neg4(2)	0.0524	272.852	31.014	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	0(4)					
1S	2.26(3)	7(5)					
1S	2.46(5)	3(5)					
1Br	2.40(5)	1(5)					
1Imd	2.00(4)	3(4)	neg1(2)	0.0546	284.469	32.334	11
0N/O							
1S	2.24(2)	4(4)					
1S	2.38(4)	2(5)					
1Br	2.33(5)	2(6)					
1Imd	1.95(0.16)	10(19)					
1Imd	1.99(8)	2(4)	neg4(3)	0.0596	310.652	35.310	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.27(3)	6(4)	0(2)	0.0529	275.555	31.321	11

1S	2.46(5)	3(4)					
1Br	2.41(4)	1(5)					
1Imd	2.01(4)	3(4)					
0N/O							
1S	2.24(2)	3(3)					
1S	2.38(4)	2(5)					
1Br	2.33(5)	3(5)					
1Imd	1.95(0.15)	10(18)					
1Imd	1.99(7)	2(4)	neg4(3)	0.058	302.421	34.374	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.27(3)	6(3)					
1S	2.47(5)	2(4)					
1Br	2.41(4)	2(5)					
1Imd	2.01(4)	3(4)	0(2)	0.0522	271.810	30.895	11
0N/O							
1S	2.24(2)	3(3)					
1S	2.38(4)	2(4)					
1Br	2.36(4)	3(5)					
1Imd	1.95(0.15)	10(17)					
1Imd	1.99(7)	2(4)	neg4(3)	0.057	296.730	33.728	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	1(4)					
1S	2.27(3)	5(3)					
1S	2.46(5)	2(4)					
1Br	2.41(4)	2(5)					
1Imd	2.01(4)	3(4)	0(2)	0.0515	268.106	30.474	11
0N/O							
1S	2.24(3)	2(3)					
1S	2.41(6)	8(7)					
1Br	2.75(4)	10(4)					
1Imd	2.01(5)	0(3)					
1Imd	1.95(0.10)	7(12)	neg3(3)	0.0728	379.538	43.140	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(3)	0(3)					
1S	2.25(4)	7(5)					
1S	2.46(5)	3(4)					
1Br	2.41(4)	0(4)					
1Imd	1.99(4)	3(4)	neg1(2)	0.053	275.972	31.368	11

0N/O							
1S	2.23(2)	4(4)					
1S	2.39(5)	2(6)					
1Br	2.34(5)	2(6)					
1Imd	1.93(0.11)	10(18)					
1Imd	1.99(6)	1(3)	neg4(3)	0.0606	315.843	35.900	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	0(3)					
1S	2.26(3)	7(4)					
1S	2.47(4)	3(4)					
1Br	2.42(4)	1(4)					
1Imd	2.00(4)	3(4)	neg1(2)	0.0514	267.759	30.435	11
0N/O							
1S	2.24(2)	4(3)					
1S	2.40(4)	2(5)					
1Br	2.35(5)	2(6)					
1Imd	1.99(6)	1(3)					
1Imd	1.94(0.12)	10(17)	neg4(3)	0.0587	305.593	34.735	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.26(3)	6(4)					
1S	2.47(4)	3(4)					
1Br	2.42(4)	2(4)					
1Imd	2.01(4)	3(4)	neg1(2)	0.0507	264.209	30.031	11
0N/O							
1S	2.24(2)	3(3)					
1S	2.40(4)	2(5)					
1Br	2.35(5)	3(5)					
1Imd	1.99(6)	1(3)					
1Imd	1.94(0.12)	10(17)	neg4(2)	0.0574	299.244	34.013	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.26(3)	6(3)					
1S	2.47(4)	2(4)					
1Br	2.42(4)	2(4)					
1Imd	2.01(4)	3(4)	neg1(2)	0.0501	260.872	29.652	11
0N/O							
1S	2.24(2)	3(3)					
1S	2.40(4)	1(5)					
1Br	2.35(4)	3(5)	neg4(2)	0.0563	293.325	33.341	11

1Imd	1.94(0.12)	10(17)					
1Imd	1.99(6)	1(3)					

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	0(3)					
1S	2.26(4)	8(6)					
1S	2.46(5)	4(4)					
1Br	2.40(4)	0(4)					
1Imd	1.99(4)	3(4)	neg1(2)	0.0552	287.554	32.685	11
0N/O							
1S	2.24(2)	4(4)					
1S	2.39(4)	2(6)					
1Br	2.33(5)	2(6)					
1Imd	1.98(7)	1(3)					
1Imd	1.94(0.14)	10(19)	neg4(3)	0.0616	320.710	36.453	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	0(3)					
1S	2.27(3)	7(5)					
1S	2.46(5)	3(4)					
1Br	2.41(4)	1(4)					
1Imd	2.00(4)	3(4)	neg1(2)	0.0537	279.713	31.793	11
0N/O							
1S	2.24(2)	4(4)					
1S	2.39(4)	2(5)					
1Br	2.34(4)	2(6)					
1Imd	1.94(0.13)	10(18)					
1Imd	1.99(6)	1(3)	neg4(3)	0.0598	311.609	35.419	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	0(4)					
1S	2.27(3)	6(4)					
1S	2.47(5)	3(4)					
1Br	2.41(4)	2(5)					
1Imd	2.00(4)	3(4)	neg1(2)	0.053	276.355	31.412	11
0N/O							
1S	2.24(2)	3(3)					
1S	2.39(4)	2(5)					
1Br	2.34(4)	3(5)					
1Imd	1.99(6)	2(3)					
1Imd	1.94(0.13)	10(17)	neg4(3)	0.0587	305.675	34.744	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	1(4)					
1S	2.27(3)	6(3)					
1S	2.47(5)	2(4)					
1Br	2.41(4)	2(5)					
1Imd	2.00(4)	3(4)	neg1(2)	0.0523	272.733	31.000	11
0N/O							
1S	2.24(2)	3(3)					
1S	2.39(4)	2(5)					
1Br	2.34(4)	3(5)					
1Imd	1.95(0.13)	10(17)					
1Imd	1.99(6)	2(3)	neg4(3)	0.0576	299.900	34.088	11

Table G.9. Additional Fits for Co(II) E63C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.12(3)	2(2)	4(5)	0.2545	2429.818	357.490	3
3N/O	2.12(2)	4(2)	2(4)	0.1632	1557.656	229.172	3
4N/O	2.11(2)	7(2)	1(3)	0.1264	1207.176	177.607	3
5N/O	2.10(2)	8(2)	0(3)	0.1217	1161.507	170.888	3
6N/O	2.10(2)	10(2)	neg1(3)	0.1353	1291.787	190.056	3
7N/O	2.09(3)	12(2)	neg2(3)	0.1590	1517.584	223.277	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.22(3)	6(2)	neg16(6)	0.1813	1730.691	254.630	3
3S	2.22(3)	9(1)	neg17(5)	0.1283	1224.909	180.217	3
4S	2.21(2)	12(1)	neg18(4)	0.1135	1083.773	159.452	3
5S	2.21(3)	14(1)	neg19(4)	0.1165	1112.035	163.610	3
6S	2.21(3)	16(2)	neg20(4)	0.1279	1221.159	179.665	3
7S	2.21(3)	17(2)	neg20(5)	0.1432	1367.531	201.200	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.03(1)	1(1)					
1N/O	2.16(1)	5(1)	neg2(2)	0.0213	202.873	42.293	5
2N/O	2.00(1)	0(1)					
2N/O	2.15(1)	2(1)	neg3(2)	0.0265	252.687	52.677	5
3N/O	2.04(1)	3(1)					
1N/O	2.17(1)	4(1)	neg3(1)	0.0209	199.767	41.645	5

4N/O	2.04(2)	5(1)					
1N/O	2.16(1)	3(1)	neg4(2)	0.0425	405.962	84.631	5
3N/O	2.01(2)	3(2)					
2N/O	2.15(1)	1(1)	neg4(2)	0.0532	508.280	105.961	5
5N/O	2.04(2)	8(2)					
1N/O	2.16(2)	2(2)	neg5(3)	0.0722	689.456	143.730	5
4N/O	2.01(3)	7(3)					
2N/O	2.15(2)	1(2)	neg5(3)	0.0866	826.411	172.281	5
3N/O	1.99(3)	5(3)					
3N/O	2.13(2)	2(2)	neg5(3)	0.0980	935.434	195.009	5
6N/O	2.04(3)	12(3)					
1N/O	2.15(3)	1(2)	neg5(3)	0.1023	976.177	203.503	5
5N/O	2.02(4)	11(5)					
2N/O	2.14(3)	2(3)	neg6(4)	0.1167	1114.256	232.288	5
4N/O	1.99(5)	11(7)					
3N/O	2.12(3)	4(3)	neg6(4)	0.1277	1218.744	254.070	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.22(2)	2(1)					
1S	2.08(3)	1(2)	neg23(5)	0.0747	713.457	148.734	5
2S	2.09(3)	6(3)					
2S	2.23(3)	4(2)	neg24(5)	0.0807	770.565	160.639	5
3S	2.22(3)	9(2)					
1S	3.00(0.16)	14(23)	neg17(5)	0.1106	1055.939	220.131	5
4S	2.21(3)	11(2)					
1S	1.54(0.24)	36(46)	neg19(6)	0.1084	1034.585	215.679	5
3S	2.23(3)	9(2)					
2S	2.41(0.12)	22(26)	neg14(7)	0.1034	987.156	205.791	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.24(3)	10(1)					
2S	2.49(5)	14(7)	neg12(4)	0.0844	806.126	168.052	5
3S	2.40(0.10)	25(23)					
3S	2.23(3)	9(2)	neg14(7)	0.0997	951.522	198.363	5

6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.24(3)	10(1)					
3S	2.48(5)	18(8)	neg11(4)	0.0784	748.801	156.102	5

Co-N(2.0) Co-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.99(3)	3(2)					5
1S	2.25(2)	1(1)	neg12(4)	0.0650	620.412	129.337	
1N/O	3.16(4)	7(3)					5
2S	2.21(3)	6(2)	neg18(6)	0.1436	1370.914	285.793	
2N/O	1.96(5)	7(4)					
2S	2.24(3)	6(2)	neg15(5)	0.0849	810.523	168.969	5
3N/O	2.00(4)	7(2)					
1S	2.26(2)	2(1)	neg11(4)	0.0647	617.279	128.683	5
1N/O	1.92(5)	4(4)					
3S	2.23(3)	9(2)	neg18(5)	0.0929	886.459	184.799	5
1N/O	1.88(0.33)	19(45)					
4S	2.21(4)	11(3)	neg19(8)	0.1085	1035.813	215.935	5
4N/O	2.03(5)	11(3)					
1S	2.26(2)	3(2)	neg10(5)	0.0681	650.015	135.508	5
2N/O	1.95(0.17)	15(12)					
3S	2.23(4)	10(3)	neg17(8)	0.1023	976.941	203.662	5
3N/O	1.99(0.10)	14(6)					
2S	2.24(3)	7(2)	neg14(7)	0.0909	868.268	181.007	5
5N/O	2.06(7)	15(4)					
1S	2.26(2)	4(2)	neg7(6)	0.0694	662.737	138.160	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.02(0.14)	18(7)					
2S	2.24(3)	8(3)	neg12(9)	0.0922	880.155	183.485	5
2N/O	1.87(0.30)	27(50)	neg19(8)	0.1072	1023.655	213.400	5

4S	2.21(4)	11(2)					
3N/O	1.97(0.25)	23(16)					
3S	2.22(4)	10(3)	neg16(10)	0.1026	979.585	204.213	5
6N/O	2.10(8)	17(5)					
1S	2.26(2)	5(2)	neg5(7)	0.0680	648.805	135.256	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.06(0.16)	21(11)					
2S	2.24(4)	8(3)	neg11(11)	0.0915	873.066	182.007	5
2N/O	2.71(5)	5(5)					
5S	2.22(2)	13(1)	neg17(4)	0.0821	784.010	163.442	5
4N/O	1.99(0.29)	28(17)					
3S	2.22(4)	10(2)	neg16(11)	0.1021	974.703	203.195	5
3N/O	1.87(0.30)	33(52)					
4S	2.21(4)	11(2)	neg20(9)	0.1065	1017.074	212.029	5

Co-N(2.0) Co-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(4)	3(3)					5
1Br	2.44(7)	13(8)	2(7)	0.2158	2059.899	429.425	
1N/O	2.12(6)	1(3)					5
2Br	2.47(0.12)	18(11)	4(14)	0.3832	3658.677	762.721	
2N/O	2.12(4)	3(3)					
2Br	2.46(9)	20(10)	3(7)	0.2165	2066.413	430.783	5
3N/O	2.11(3)	5(2)					
1Br	2.43(5)	13(6)	1(4)	0.1299	1240.097	258.522	5
1N/O	2.13(5)	1(3)					
3Br	2.49(0.13)	22(12)	4(13)	0.3800	3627.684	756.260	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(3)	8(2)					
1Br	2.41(4)	13(5)	0(3)	0.0894	853.244	177.875	5
2N/O	2.12(4)	3(3)					
3Br	2.48(9)	24(12)	3(6)	0.2156	2058.419	429.117	5
3N/O	2.12(3)	5(2)	1(4)	0.1325	1265.035	263.721	5

2Br	2.44(7)	20(9)					
5N/O	2.11(3)	10(2)					
1Br	2.40(3)	12(4)	neg1(3)	0.0746	712.558	148.546	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.12(2)	7(2)					
2Br	2.42(5)	20(7)	1(3)	0.0942	899.347	187.486	5
2N/O	2.12(4)	3(3)					
4Br	2.49(9)	27(12)	3(6)	0.2148	2050.924	427.554	5
3N/O	2.12(3)	5(2)					
3Br	2.45(7)	25(10)	2(4)	0.1330	1270.182	264.794	5
6N/O	2.11(3)	12(2)					
1Br	2.40(3)	11(3)	neg2(3)	0.0743	709.324	147.872	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.11(2)	9(2)					
2Br	2.41(4)	18(5)	0(3)	0.0826	788.311	164.338	5
2N/O	2.13(3)	3(3)					
5Br	2.49(0.10)	30(13)	3(6)	0.2142	2044.851	426.288	5
4N/O	2.12(2)	7(2)					
3Br	2.43(5)	24(8)	1(3)	0.0958	914.769	190.701	5
3N/O	2.12(3)	5(2)					
4Br	2.46(7)	28(11)	2(4)	0.1334	1273.480	265.481	5

Co-N(2.0) Co-S(2.2) Co-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(4)	9(3)					
1S	2.29(4)	1(3)					
1Br	2.26(6)	8(6)	neg7(4)	0.0381	363.909	130.113	7
3N/O	2.02(5)	8(4)					
2S	2.34(6)	7(6)					
1Br	2.34(5)	6(3)	neg8(5)	0.0453	432.890	154.776	7
3N/O	2.02(4)	4(2)					
1S	2.27(3)	0(2)					
2Br	2.21(7)	15(7)	neg9(4)	0.0327	311.770	111.471	7
2N/O	2.01(5)	4(3)	neg11(4)	0.0381	364.140	130.195	7

2S	2.27(4)	2(2)
2Br	2.24(6)	11(6)

Table G.10. Additional Fits for Co(II) E63C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(2)	2(2)	4(4)	0.3152	5634.792	335.447	3
3N/O	2.12(2)	5(1)	2(3)	0.2287	2377.836	141.556	3
4N/O	2.11(2)	7(1)	1(2)	0.1935	2011.959	119.775	3
5N/O	2.11(2)	9(1)	0(2)	0.1885	1960.407	116.706	3
6N/O	2.10(2)	10(2)	neg1(2)	0.2011	2091.495	124.510	3
7N/O	2.10(2)	12(2)	neg2(2)	0.2233	2321.971	138.230	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.22(2)	6(1)	neg15(5)	0.2425	2521.839	150.129	3
3S	2.22(2)	9(1)	neg17(4)	0.1937	2014.559	119.930	3
4S	2.21(2)	12(1)	neg18(4)	0.1802	1874.225	111.575	3
5S	2.21(2)	14(1)	neg19(4)	0.1831	1904.540	113.380	3
6S	2.21(2)	16(1)	neg20(4)	0.1939	2016.249	120.030	3
7S	2.21(3)	17(1)	neg20(4)	0.2082	2165.469	128.913	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.03(1)	1(1)					
1N/O	2.17(1)	5(1)	neg2(2)	0.0706	733.728	49.583	5
2N/O	2.00(1)	0(1)					
2N/O	2.15(1)	2(1)	neg3(2)	0.0819	851.577	57.547	5
3N/O	2.04(1)	2(1)					
1N/O	2.17(1)	4(1)	neg3(2)	0.0743	772.474	52.202	5
4N/O	2.04(1)	5(1)					
1N/O	2.17(1)	3(1)	neg4(2)	0.0994	1033.682	69.854	5
3N/O	2.01(1)	3(1)					
2N/O	2.15(1)	1(1)	neg4(2)	0.1121	1165.701	78.775	5
5N/O	2.04(2)	8(2)					
1N/O	2.16(1)	2(1)	neg5(2)	0.1324	1376.964	93.052	5
4N/O	2.01(2)	6(2)					
2N/O	2.15(2)	0(1)	neg5(2)	0.1490	1549.556	104.715	5

3N/O	1.99(2)	4(2)					
3N/O	2.14(2)	2(1)	neg5(2)	0.1622	1686.714	113.984	5
6N/O	2.04(2)	11(2)					
1N/O	2.15(2)	1(1)	neg5(2)	0.1657	1723.102	116.443	5
5N/O	2.02(3)	10(3)					
2N/O	2.14(2)	2(2)	neg6(2)	0.1830	1903.381	128.626	5
4N/O	1.99(3)	10(4)					
3N/O	2.13(2)	4(2)	neg6(3)	0.1960	2037.943	137.719	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.22(2)	2(1)					
1S	2.08(2)	1(1)	neg23(3)	0.1298	1350.274	91.248	5
2S	2.09(2)	6(2)					
2S	2.23(2)	3(1)	neg24(4)	0.1405	1460.586	98.703	5
3S	2.22(2)	9(1)					
1S	3.06(4)	6(4)	neg16(3)	0.1656	1722.503	116.402	5
4S	2.21(3)	11(1)					
1S	1.55(0.19)	36(35)	neg19(5)	0.1755	1825.437	123.358	5
3S	2.22(2)	6(2)					
2S	2.08(3)	7(2)	neg24(4)	0.1564	1626.814	109.936	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.25(2)	10(1)					
2S	2.49(4)	13(5)	neg11(3)	0.1504	1564.486	105.724	5
3S	2.22(2)	7(2)					
3S	2.09(4)	12(5)	neg25(4)	0.1699	1767.222	119.424	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.22(2)	14(1)					
2S	3.04(5)	14(7)	neg17(3)	0.1502	1562.069	105.561	5
4S	2.24(2)	10(1)					
3S	2.49(4)	17(6)	neg11(3)	0.1452	1509.812	102.029	5

Co-N(2.0) Co-S(2.2)							
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.99(2)	3(1)					5
1S	2.26(1)	1(1)	neg12(3)	0.1193	1240.296	83.816	
1N/O	1.94(2)	1(2)					5
2S	2.23(2)	5(1)	neg16(3)	0.1326	1379.370	93.214	
2N/O	1.96(4)	6(3)					
2S	2.24(2)	6(1)	neg15(4)	0.1476	1535.386	103.757	5
3N/O	2.00(3)	7(2)					
1S	2.26(2)	2(1)	neg11(3)	0.1238	1287.091	86.978	5
1N/O	1.93(3)	3(3)					
3S	2.23(2)	8(1)	neg17(4)	0.1566	1628.333	110.038	5
1N/O	1.34(8)	13(11)					
4S	2.21(2)	11(1)	neg18(4)	0.1754	1824.273	123.280	5
4N/O	2.02(4)	11(2)					
1S	2.26(2)	3(1)	neg10(4)	0.1308	1360.539	91.942	5
2N/O	1.96(0.12)	14(9)					
3S	2.23(3)	10(2)	neg16(6)	0.1689	1756.386	118.692	5
3N/O	1.99(7)	12(4)					
2S	2.24(2)	7(2)	neg14(5)	0.1562	1624.538	109.782	5
5N/O	2.05(6)	15(3)					
1S	2.26(2)	4(2)	neg8(5)	0.1348	1401.418	94.704	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.02(0.10)	17(6)					
2S	2.24(3)	8(2)	neg12(7)	0.1582	1645.568	111.203	5
2N/O	1.88(0.26)	28(40)					
4S	2.21(3)	12(2)	neg19(7)	0.1750	1819.521	122.958	5
3N/O	1.98(0.19)	23(12)					
3S	2.23(3)	10(2)	neg16(7)	0.1696	1763.290	119.159	5
6N/O	2.09(7)	18(4)					
1S	2.26(2)	4(2)	neg5(6)	0.1353	1406.560	95.052	5
1N/O	4.16(6)	2(5)					
6S	2.21(2)	16(1)	neg20(4)	0.1822	1894.667	128.037	5

5N/O	2.06(0.12)	21(8)					
2S	2.24(3)	8(2)	neg11(9)	0.1578	1641.260	110.912	5
2N/O	2.69(3)	4(3)					
5S	2.22(2)	13(1)	neg17(3)	0.1536	1597.131	107.930	5
4N/O	2.00(0.21)	28(14)					
3S	2.23(3)	10(2)	neg16(8)	0.1692	1759.286	118.888	5
3N/O	1.89(0.27)	34(43)					
4S	2.21(3)	12(2)	neg19(7)	0.1745	1814.722	122.634	5

Co-N(2.0) Co-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.12(3)	3(2)					5
1Br	2.44(5)	13(6)	2(5)	0.2809	2920.835	197.382	
1N/O	2.13(4)	0(2)					5
2Br	2.48(8)	19(7)	4(8)	0.4372	4545.914	307.201	
2N/O	2.12(3)	3(2)					
2Br	2.47(6)	20(7)	3(4)	0.2781	2891.624	195.408	5
3N/O	2.11(2)	5(2)					
1Br	2.43(4)	14(5)	1(3)	0.1983	2061.989	139.344	5
1N/O	1.88(4)	2(3)					
3Br	2.28(3)	11(1)	neg39(8)	0.2884	2998.957	202.662	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(2)	8(2)					
1Br	2.41(3)	13(4)	0(3)	0.1593	1656.747	111.959	5
2N/O	2.12(2)	3(2)					
3Br	2.48(6)	24(8)	3(4)	0.2760	2870.182	193.959	5
3N/O	2.12(2)	5(2)					
2Br	2.45(5)	21(7)	1(3)	0.1983	2062.296	139.365	5
5N/O	2.11(2)	10(2)					
1Br	2.40(2)	11(3)	neg1(2)	0.1449	1506.695	101.818	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.12(2)	7(2)					
2Br	2.43(4)	20(5)	1(2)	0.1621	1685.717	113.916	5

2N/O	2.12(2)	3(2)					
4Br	2.49(6)	27(8)	3(4)	0.2750	2860.156	193.282	5
3N/O	2.12(2)	5(2)					
3Br	2.46(5)	25(7)	2(3)	0.1977	2056.181	138.951	5
6N/O	2.11(2)	12(2)					
1Br	2.39(2)	10(20	neg2(2)	0.1441	1498.463	101.262	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.11(2)	9(2)					
2Br	2.42(3)	19(4)	0(2)	0.1512	1572.144	106.241	5
2N/O	2.12(2)	3(2)					
5Br	2.49(6)	29(8)	3(4)	0.2747	2857.037	193.071	5
4N/O	2.12(2)	7(2)					
3Br	2.44(4)	24(6)	1(2)	0.1624	1689.276	114.157	5
3N/O	2.12(2)	5(2)					
4Br	2.47(5)	27(7)	2(3)	0.1977	2056.120	138.947	5

Co-N(2.0) Co-S(2.2) Co-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(3)	9(2)					
1S	2.29(2)	0(2)					
1Br	2.26(4)	6(3)	neg6(3)	0.0922	958.833	74.921	7
3N/O	2.01(3)	7(2)					
2S	2.35(4)	6(4)					
1Br	2.34(3)	5(2)	neg8(3)	0.1040	1081.601	84.514	7
3N/O	2.02(3)	3(2)					
1S	2.27(2)	0(1)					
2Br	2.21(4)	14(5)	neg9(3)	0.0859	893.571	69.822	7
2N/O	2.02(3)	4(2)					
2S	2.27(3)	2(2)					
2Br	2.24(4)	10(3)	neg10(3)	0.0923	959.678	74.987	7

Co-N(2.0) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(3)	10(3)					
1Imd	2.06(9)	9(11)	neg1(2)	0.1638	2928.667	197.912	5
4N/O	2.10(2)	12(3)					
1Imd	2.15(1)	3(1)					
1Imd	2.00(2)	1(1)	neg2(1)	0.0745	774.576	60.524	7

3N/O	2.10(1)	5(1)					
1Imd	1.99(1)	3(1)					
1Imd	2.14(1)	3(1)					
1Imd	1.88(3)	7(6)	neg4(1)	0.0374	389.403	36.063	9
2N/O	2.11(1)	2(2)					
1Imd	2.22(0.49)	36(128)					
1Imd	2.15(2)	3(2)					
1Imd	1.93(8)	11(13)					
1Imd	1.99(2)	2(2)	neg3(3)	0.0354	367.951	41.823	11
1N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13
4N/O	2.12(1)	4(1)					
1Imd	1.97(2)	0(1)	neg3(2)	0.1355	1408.676	95.195	5
3N/O	2.11(1)	6(2)					
1Imd	1.99(1)	1(1)					
1Imd	2.15(1)	2(1)	neg2(1)	0.0507	526.808	41.164	7
2N/O	2.11(1)	2(1)					
1Imd	1.94(5)	10(11)					
1Imd	1.99(2)	2(1)					
1Imd	2.15(1)	3(2)	neg3(1)	0.0357	371.596	34.414	9
1N/O	2.11(2)	1(2)					
1Imd	2.19(0.39)	21(87)					
1Imd	2.16(5)	3(4)					
1Imd	2.00(7)	2(3)					
1Imd	1.99(0.23)	8(36)	neg2(3)	0.0496	516.267	58.681	11
0N/O							
1Imd	2.06(5)	17(6)					
1Imd	1.96(5)	15(6)					
1Imd	1.87(6)	6(8)					
1Imd	2.17(5)	16(7)					
1Imd	2.27(6)	10(10)	neg3(2)	0.1442	1499.571	170.447	11
3N/O	2.12(1)	2(1)					
1Imd	1.98(2)	0(1)	neg2(2)	0.1286	1337.693	90.398	5
2N/O	2.11(1)	2(1)					
1Imd	1.99(1)	2(1)					
1Imd	2.15(1)	2(1)	neg1(1)	0.0413	429.120	33.531	7

1N/O	2.11(1)	1(1)					
1Imd	2.17(5)	2(3)					
1Imd	2.01(0.10)	1(6)					
1Imd	2.02(0.19)	5(24)	neg2(2)	0.0524	545.405	50.510	9
0N/O							
1Imd	2.02(0.15)	5(23)					
1Imd	2.19(0.38)	1(68)					
1Imd	2.14(0.24)	6(18)					
1Imd	1.95(0.16)	0(26)	neg2(3)	0.1578	1640.857	151.961	9
2N/O	2.13(1)	1(1)					
1Imd	1.99(2)	1(1)	neg2(2)	0.1577	1640.264	110.845	5
1N/O	2.12(2)	1(2)					
1Imd	2.15(2)	3(1)					
1Imd	2.00(1)	3(1)	neg1(1)	0.0722	750.464	58.640	7
0N/O							
1Imd	2.07(3)	7(6)					
1Imd	2.18(3)	6(4)					
1Imd	1.97(3)	4(5)	neg2(2)	0.1703	1771.252	138.402	7

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(4)	16(6)					
1S	2.26(1)	2(1)					
1Imd	1.99(2)	2(1)	neg6(3)	0.0710	1268.964	99.154	7
3N/O	2.13(3)	3(1)					
1S	2.18(4)	9(8)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(1)	2(1)	neg2(1)	0.0298	309.507	28.664	9
2N/O	2.14(4)	2(2)					
1S	2.22(4)	9(9)					
1Imd	1.99(2)	2(2)					
1Imd	2.13(3)	2(4)					
1Imd	2.24(7)	5(13)	neg1(2)	0.0301	313.324	35.614	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(4)	15(6)					
1S	2.26(1)	3(1)					
1Imd	1.98(2)	2(2)	neg6(3)	0.0752	782.028	61.106	7
3N/O	2.04(5)	10(4)					
1S	2.25(1)	2(1)					
1Imd	1.95(2)	1(2)	neg12(3)	0.0611	635.376	58.843	9

1Imd	1.76(4)	8(5)					
2N/O	2.14(3)	2(2)					
1S	2.22(4)	11(9)					
1Imd	2.24(8)	6(15)					
1Imd	1.99(2)	3(2)					
1Imd	2.13(3)	2(4)	neg1(2)	0.0327	340.360	38.687	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.13(4)	15(6)					
1S	2.26(1)	3(1)					
1Imd	1.98(2)	2(2)	neg6(3)	0.0791	822.800	64.292	7
3N/O	2.13(2)	4(1)					
1S	2.18(4)	12(8)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(1)	2(1)	neg2(1)	0.0333	346.294	32.071	9
2N/O	2.13(3)	2(2)					
1S	2.22(4)	12(10)					
1Imd	2.13(3)	2(4)					
1Imd	2.24(8)	7(18)					
1Imd	1.98(2)	2(2)	neg1(2)	0.0349	362.721	41.228	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	8(3)					
1S	2.72(8)	17(12)					
1Imd	2.10(9)	9(11)	0(2)	0.1400	1455.748	113.749	7
3N/O	2.10(1)	6(2)					
1S	2.68(7)	22(11)					
1Imd	2.15(1)	2(1)					
1Imd	1.99(2)	1(1)	neg1(1)	0.0469	487.956	45.190	9
2N/O	2.11(2)	2(1)					
1S	2.34(0.16)	42(48)					
1Imd	1.93(7)	9(11)					
1Imd	1.99(2)	3(2)					
1Imd	2.14(2)	3(2)	neg4(2)	0.0341	354.894	40.339	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.11(2)	8(3)					
1S	2.73(8)	17(13)					
1Imd	2.10(9)	9(11)	0(2)	0.1404	1460.197	114.097	7
3N/O	2.10(1)	6(2)	neg1(1)	0.0474	493.426	45.697	9

1S	2.69(7)	23(12)					
1Imd	1.99(2)	1(1)					
1Imd	2.15(1)	2(1)					
2N/O	2.11(1)	2(1)					
1S	2.36(0.17)	46(54)					
1Imd	2.14(2)	3(2)					
1Imd	1.99(2)	3(2)					
1Imd	1.93(7)	9(11)	neg4(2)	0.0341	354.947	40.345	11

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.13(2)	2(2)					
2S	2.22(2)	13(6)					
1Imd	1.97(2)	0(1)	neg7(3)	0.0898	933.386	72.933	7
2N/O	2.11(1)	2(1)					
2S	2.45(0.33)	67(64)					
1Imd	1.99(1)	2(1)					
1Imd	2.15(2)	2(1)	neg2(2)	0.0398	413.761	38.319	9
1N/O	2.11(2)	1(2)					
2S	2.37(8)	35(20)					
1Imd	2.15(3)	3(2)					
1Imd	1.97(0.11)	7(16)					
1Imd	2.00(4)	2(2)	neg4(2)	0.0438	455.024	51.720	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	2(2)					
2S	2.23(3)	15(6)					
1Imd	1.97(2)	0(1)	neg7(3)	0.0945	982.750	76.790	7
2N/O	2.11(1)	2(1)					
2S	2.49(0.37)	71(66)					
1Imd	2.15(2)	2(1)					
1Imd	1.99(1)	2(1)	neg2(2)	0.0398	414.096	38.350	9
1N/O	2.11(2)	1(2)					
2S	2.39(9)	38(22)					
1Imd	2.16(3)	3(2)					
1Imd	1.98(0.11)	7(16)					
1Imd	2.00(4)	2(2)	neg3(2)	0.0441	458.567	52.123	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	2(2)					
2S	2.24(3)	16(7)					
1Imd	1.97(2)	0(1)	neg7(3)	0.0984	1023.435	79.969	7

2N/O	2.11(1)	2(1)					
2S	2.52(0.38)	74(66)					
1Imd	1.99(1)	2(1)					
1Imd	2.15(2)	2(1)	neg2(2)	0.0398	413.795	38.322	9
1N/O	2.11(2)	1(2)					
2S	2.41(0.10)	40(23)					
1Imd	2.16(3)	3(2)					
1Imd	1.98(0.11)	6(16)					
1Imd	2.00(5)	2(2)	neg3(2)	0.0442	459.887	52.273	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	2(1)					
2S	2.24(3)	17(7)					
1Imd	1.97(2)	0(1)	neg7(3)	0.1019	1059.614	82.796	7
2N/O	2.11(1)	2(1)					
2S	2.55(0.39)	75(65)					
1Imd	1.99(1)	2(1)					
1Imd	2.15(2)	2(1)	neg1(2)	0.0397	413.026	38.251	9
1N/O	2.11(2)	1(2)					
2S	2.42(0.10)	42(24)					
1Imd	2.00(5)	2(2)					
1Imd	2.16(3)	3(2)					
1Imd	1.98(0.11)	6(16)	neg3(2)	0.0444	461.534	52.460	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.12(2)	2(1)					
2S	2.24(3)	18(7)					
1Imd	1.97(2)	0(1)	neg7(3)	0.1044	1085.858	84.847	7
2N/O	2.11(1)	2(1)					
2S	2.57(0.38)	77(65)					
1Imd	1.99(1)	2(1)					
1Imd	2.15(2)	2(1)	neg1(2)	0.0397	412.641	38.215	9
1N/O	2.11(2)	1(2)					
2S	2.43(0.10)	43(24)					
1Imd	1.98(0.11)	6(16)					
1Imd	2.01(5)	2(2)					
1Imd	2.16(3)	3(2)	neg3(2)	0.0444	461.808	52.491	11

Co-N(2.0) Co-S(2.2) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

3N/O	2.08(4)	13(5)					
1S	2.49(3)	8(4)					
1S	2.28(1)	2(1)					
1Imd	2.00(2)	2(2)	neg6(2)	0.0444	461.841	42.772	9
2N/O	2.12(3)	9(4)					
1S	2.52(3)	9(3)					
1S	2.28(2)	5(2)					
1Imd	2.14(2)	0(2)					
1Imd	1.98(1)	1(1)	neg3(1)	0.0177	184.485	20.969	11
1N/O	2.86(7)	7(8)					
1S	2.28(2)	4(2)					
1S	1.78(5)	26(8)					
1Imd	2.15(2)	5(2)					
1Imd	2.01(2)	4(1)					
1Imd	2.29(4)	1(4)	neg1(2)	0.0318	331.179	48.718	13

Co-N(2.0) Co-N(2.2) Co-S(2.2) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(2)					
1N/O	2.15(1)	4(1)					
1S	2.62(7)	16(7)					
1S	2.33(0.14)	31(23)					
1Imd 0°	2.01(2)	0(2)					
1Imd 0°	2.17(3)	2(3)	neg2(1)	0.0109	112.991	16.622	13
1N/O	2.01(2)	2(2)					
1N/O	2.15(1)	4(1)					
1S	2.29(0.10)	23(16)					
1S	2.61(7)	17(7)					
1Imd 0°	2.02(3)	0(2)					
1Imd 5°	2.19(4)	1(3)	neg2(1)	0.0131	135.771	19.973	13
1N/O	2.01(1)	3(1)					
1N/O	2.15(1)	5(1)					
1S	2.55(0.11)	19(11)					
1S	2.25(9)	19(15)					
1Imd 0°	2.03(4)	6(4)					
1Imd 10°	2.15(5)	5(5)	neg3(2)	0.0142	147.649	21.720	13
1N/O	2.01(1)	4(1)					
1N/O	2.15(1)	5(1)					
1S	2.11(7)	19(11)					
1S	1.78(8)	31(11)					
1Imd 5°	2.07(5)	7(5)					
1Imd 10°	2.14(5)	4(4)	neg1(2)	0.0169	175.881	25.873	13

Co-N(2.0) Co-S(2.2) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

3N/O	2.08(4)	12(5)					
1S	2.49(3)	8(3)					
1S	2.28(1)	2(1)					
1Imd	2.00(2)	2(2)	neg6(2)	0.0450	467.436	43.290	9
2N/O	2.13(3)	11(6)					
1S	2.27(1)	4(2)					
1S	2.53(3)	12(4)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg3(1)	0.0174	181.153	20.591	11
1N/O	2.11(4)	3(4)					
1S	2.28(2)	5(2)					
1S	2.55(3)	11(4)					
1Imd	1.98(1)	2(2)					
1Imd	2.12(3)	1(4)					
1Imd	2.23(6)	5(12)	neg2(1)	0.0160	166.640	24.514	13

Co-N(2.0) Co-S(2.2) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(4)	15(6)					
1S	2.27(1)	2(1)					
1S	2.50(4)	11(5)					
1Imd	1.99(2)	2(1)	neg6(2)	0.0440	457.315	42.352	9
2N/O	2.13(3)	11(6)					
1S	2.27(1)	4(2)					
1S	2.53(3)	12(4)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg3(1)	0.0173	179.614	20.416	11
1N/O	2.08(4)	2(3)					
1S	2.29(2)	4(2)					
1S	2.52(3)	10(4)					
1Imd	1.97(2)	2(1)					
1Imd	2.13(2)	1(2)					
1Imd	1.90(9)	16(14)	neg6(2)	0.0153	158.881	23.372	13

Co-N(2.0) Co-S(2.2) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(4)	16(6)					
1S	2.27(1)	2(10					
1S	2.50(4)	12(5)					
1Imd	1.99(2)	2(1)	neg6(2)	0.0438	454.967	42.135	9
2N/O	2.13(3)	11(6)					
1S	2.27(1)	4(2)					
1S	2.53(3)	13(4)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg4(1)	0.0171	177.865	20.217	11

1N/O	2.11(4)	4(5)					
1S	2.28(2)	5(2)					
1S	2.55(3)	12(4)					
1Imd	2.12(3)	1(4)					
1Imd	2.22(6)	5(13)					
1Imd	1.98(1)	2(2)	neg3(1)	0.0160	166.123	24.438	13

Co-N(2.0) Co-S(2.3) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(4)	13(5)					
1S	2.49(3)	8(4)					
1S	2.28(1)	2(1)					
1Imd	1.99(2)	2(2)	neg6(2)	0.0452	470.456	43.569	9
2N/O	2.13(3)	9(5)					
1S	2.27(1)	3(2)					
1S	2.53(3)	11(3)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg3(1)	0.0179	186.415	21.189	11
1N/O	2.11(4)	2(3)					
1S	2.29(3)	5(2)					
1S	2.55(3)	10(3)					
1Imd	1.97(1)	2(2)					
1Imd	2.11(4)	1(4)					
1Imd	2.22(7)	6(14)	neg3(1)	0.0165	171.543	25.235	13

Co-N(2.0) Co-S(2.3) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(4)	14(5)					
1S	2.27(1)	2(1)					
1S	2.50(4)	10(4)					
1Imd	1.99(2)	2(1)	neg6(2)	0.0444	461.600	42.749	9
2N/O	2.13(3)	9(5)					
1S	2.27(1)	4(2)					
1S	2.53(3)	11(3)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg4(1)	0.0178	185.061	21.035	11
1N/O	2.08(4)	2(3)					
1S	2.29(2)	4(2)					
1S	2.53(3)	9(3)					
1Imd	1.97(2)	2(1)					
1Imd	2.13(2)	1(2)					
1Imd	1.91(9)	16(15)	neg6(2)	0.5500	161.394	23.742	13

Co-N(2.0) Co-S(2.3) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

3N/O	2.09(4)	15(5)					
1S	2.27(1)	2(1)					
1S	2.50(4)	11(4)					
1Imd	1.99(2)	2(1)	neg6(2)	0.0442	459.382	42.544	9
2N/O	2.13(3)	10(5)					
1S	2.27(1)	4(2)					
1S	2.53(3)	12(3)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg4(1)	0.0176	183.389	20.845	11
1N/O	2.08(4)	2(3)					
1S	2.29(2)	4(2)					
1S	2.53(3)	10(3)					
1Imd	1.91(9)	16(15)					
1Imd	2.13(2)	1(2)					
1Imd	1.97(2)	2(1)	neg6(2)	0.0153	158.841	23.366	13

Co-N(2.0) Co-S(2.4) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(4)	14(5)					
1S	2.27(1)	2(1)					
1S	2.50(3)	10(4)					
1Imd	1.99(2)	2(1)	neg6(2)	0.0450	468.428	43.382	9
2N/O	2.13(3)	8(5)					
1S	2.27(2)	5(2)					
1S	2.53(3)	11(3)					
1Imd	2.14(2)	0(2)					
1Imd	1.98(1)	1(1)	neg4(1)	0.0184	190.954	21.705	11
1N/O	2.08(4)	1(3)					
1S	2.30(2)	4(3)					
1S	2.53(3)	9(3)					
1Imd	2.13(2)	1(2)					
1Imd	1.92(0.10)	16(16)					
1Imd	1.97(2)	2(1)	neg6(2)	0.0159	165.078	24.284	13

Co-N(2.0) Co-S(2.4) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(4)	14(5)					
1S	2.27(1)	2(1)					
1S	2.50(3)	10(4)					
1Imd	1.99(2)	2(1)	neg6(2)	0.0448	466.143	43.170	9
2N/O	2.13(3)	8(5)					
1S	2.27(2)	5(2)					
1S	2.53(3)	11(3)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg4(1)	0.0182	189.316	21.518	11

1N/O	2.08(4)	1(3)					
1S	2.29(2)	5(2)					
1S	2.53(3)	9(3)					
1Imd	1.97(2)	2(1)					
1Imd	2.13(2)	1(2)					
1Imd	1.91(0.10)	16(15)	neg6(2)	0.0156	162.326	23.879	13

Co-N(2.0) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(4)	13(5)					
1S	2.50(3)	9(4)					
1S	2.28(1)	2(1)					
1Imd	1.99(2)	2(2)	neg7(2)	0.0459	477.533	44.225	9
2N/O	2.12(2)	7(4)					
1S	2.54(3)	10(3)					
1S	2.28(2)	6(3)					
1Imd	1.98(1)	1(1)					
1Imd	2.14(2)	0(2)	neg5(1)	0.0196	203.356	23.114	11
1N/O	2.11(3)	1(3)					
1S	2.55(3)	9(3)					
1S	2.30(3)	6(3)					
1Imd	1.97(1)	2(2)					
1Imd	2.11(5)	1(5)					
1Imd	2.21(8)	6(17)	neg3(1)	0.0181	188.060	27.665	13

Table G.11. Additional Fits for Zn(II) E63C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.14(4)	2(3)	12(7)	0.3797	4913.032	722.837	3
3N/O	2.13(3)	4(3)	11(5)	0.2868	3711.763	546.099	3
4N/O	2.12(3)	6(3)	9(4)	0.2551	3301.710	485.769	3
5N/O	2.11(3)	8(3)	8(4)	0.2620	3390.374	498.814	3
6N/O	2.11(4)	10(3)	7(4)	0.2913	3769.118	554.537	3
7N/O	2.10(4)	12(3)	6(4)	0.3327	4305.477	633.449	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.26(3)	6(2)	neg3(6)	0.2061	2667.286	392.428	3
3S	2.24(2)	8(1)	neg5(4)	0.1357	1756.040	258.360	3
4S	2.24(2)	10(1)	neg6(4)	0.1159	1499.907	220.676	3
5S	2.24(2)	12(2)	neg7(4)	0.1228	1588.948	233.776	3
6S	2.23(3)	14(2)	neg8(4)	0.1438	1861.274	273.843	3
7S	2.23(3)	16(2)	neg9(4)	0.1720	2226.146	327.525	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.06(3)	2(2)					
1N/O	2.20(2)	6(2)	9(3)	0.1468	1899.593	396.006	5
2N/O	2.03(3)	1(2)					
2N/O	2.17(2)	2(2)	7(3)	0.1683	2178.394	454.128	5
3N/O	2.06(3)	1(2)					
1N/O	2.20(2)	5(2)	8(3)	0.1516	1961.779	408.970	5
4N/O	2.06(3)	4(3)					
1N/O	2.19(3)	3(3)	5(3)	0.1894	2451.264	511.013	5
3N/O	2.03(3)	2(3)					
2N/O	2.18(3)	1(3)	6(3)	0.2115	2737.169	570.615	5
5N/O	2.06(4)	7(4)					
1N/O	2.19(4)	2(3)	5(4)	0.2426	3139.882	654.568	5
4N/O	2.03(4)	6(5)					
2N/O	2.17(4)	0(4)	5(4)	0.2670	3455.651	720.396	5
3N/O	2.01(5)	4(6)					
3N/O	2.16(4)	2(4)	4(4)	0.2863	3704.986	772.375	5
6N/O	2.06(5)	10(5)					
1N/O	2.18(5)	1(5)	4(4)	0.2989	3868.646	806.493	5
5N/O	2.04(8)	12(11)					
2N/O	2.15(7)	3(6)	4(5)	0.3182	4117.722	858.418	5
4N/O	2.46(2)	2(1)					
3N/O	2.02(3)	6(2)	neg9(5)	0.0642	830.932	173.224	5

Zn-S(2.2) Zn-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(2)	3(1)					
1S	2.30(2)	1(1)	neg8(3)	0.0449	581.002	121.121	5
2S	2.14(2)	4(2)					
2S	2.28(2)	2(1)	neg9(3)	0.0572	740.292	154.328	5
3S	2.17(2)	7(2)					
1S	2.30(2)	0(1)	neg10(3)	0.0526	680.745	141.914	5
4S			No Fit	No Fit	No Fit	No Fit	5

1S							
3S	2.15(3)	8(3)					
2S	2.28(3)	4(2)	neg11(4)	0.0850	1100.083	229.333	5
5S	2.24(2)	13(1)					
1S	2.61(2)	3(2)	neg9(3)	0.0280	361.707	75.405	5
4S	2.26(3)	7(3)					
2S	2.10(5)	7(4)	neg11(5)	0.1145	1482.290	309.012	5
3S	2.13(5)	10(5)					
3S	2.26(3)	7(3)	neg11(5)	0.1221	1579.962	329.373	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.24(4)	12(2)					
2S	1.87(0.14)	38(31)	neg5(7)	0.1103	1426.739	297.431	5
4S	2.27(3)	10(1)					
3S	2.62(5)	18(8)	neg2(5)	0.0768	993.807	207.178	5

Zn-N(2.0) Zn-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.03(2)	2(1)					5
1S	2.30(2)	0(1)	2(3)	0.0473	611.802	127.542	
1N/O	1.99(2)	1(2)					5
2S	2.27(2)	4(1)	neg2(3)	0.0532	688.960	143.627	
2N/O	2.00(3)	4(2)					
2S	2.28(2)	5(1)	neg1(4)	0.0702	908.448	189.383	5
3N/O	2.04(3)	5(2)					
1S	2.31(2)	1(1)	2(3)	0.0585	757.071	157.826	5
1N/O	1.97(3)	1(3)					
3S	2.26(2)	7(1)	neg4(3)	0.0770	996.874	207.817	5
1N/O	2.09(0.24)	16(90)					
4S	2.25(4)	11(5)	neg5(8)	0.1122	1451.845	302.665	5
4N/O	2.05(4)	9(3)					
1S	2.30(2)	2(2)	3(4)	0.0852	1102.693	229.877	5
2N/O	2.04(0.12)	12(14)					
3S	2.26(4)	9(3)	neg2(7)	0.1039	1343.931	280.168	5

3N/O	2.05(8)	11(5)					
2S	2.28(3)	7(3)	1(6)	0.0935	1210.336	252.318	5
5N/O	2.08(7)	13(4)					
1S	2.30(3)	3(3)	4(6)	0.1105	1430.037	298.119	5
1N/O	2.45(2)	2(2)					
5S	2.21(3)	14(2)	neg11(4)	0.0519	672.154	140.123	5
4N/O	2.11(0.11)	15(13)					
2S	2.28(3)	7(4)	4(9)	0.0977	1264.590	263.628	5
2N/O	2.13(0.15)	20(94)					
4S	2.25(3)	11(5)	neg4(10)	0.1102	1425.475	297.167	5
3N/O	2.11(0.12)	16(29)					
3S	2.27(4)	10(5)	0(10)	0.1035	1339.114	279.164	5
6N/O	2.10(0.10)	17(5)					
1S	2.29(3)	3(3)	5(7)	0.1322	1710.534	356.593	5
1N/O	2.19(3)	2(2)					
6S	2.21(2)	11(2)	neg9(4)	0.0840	1087.007	226.607	5
5N/O	2.15(0.10)	18(15)					
2S	2.28(2)	7(3)	6(9)	0.0988	1278.474	266.522	5
2N/O	2.20(2)	1(1)					
5S	2.21(2)	8(1)	neg8(3)	0.0477	616.974	128.620	5
4N/O	2.15(9)	17(37)					
3S	2.27(3)	10(6)	2(12)	0.1004	1299.834	270.975	5
3N/O	2.15(0.12)	22(92)					
4S	2.25(3)	11(5)	neg2(14)	0.1081	1398.595	291.564	5

Zn-N(2.0) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(3)	2(2)					5
1Br	2.45(3)	5(2)	6(5)	0.1118	1446.401	301.530	
1N/O	1.41(0.26)	13(34)					5
2Br	2.32(7)	8(3)	neg24(19)	0.3730	4827.293	1006.341	
2N/O	2.07(4)	3(2)					
2Br	2.44(3)	9(2)	4(6)	0.1101	1424.872	297.042	5
3N/O	2.08(2)	5(2)					
1Br	2.45(2)	5(1)	6(3)	0.0551	713.019	148.642	5

1N/O 3Br			No Fit	No Fit	No Fit	No Fit	5
1N/O 4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 1Br	2.08(2) 2.44(1)	7(1) 6(1)	5(2)	0.0414	536.195	111.780	5
2N/O 3Br	2.06(4) 2.45(3)	4(3) 12(2)	3(6)	0.1176	1522.002	317.290	5
3N/O 2Br	2.08(3) 2.45(2)	5(2) 10(1)	5(3)	0.0580	750.897	156.539	5
5N/O 1Br	2.08(2) 2.44(2)	9(2) 6(1)	4(2)	0.0524	677.758	141.292	5
1N/O 5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 2Br	2.08(2) 2.45(2)	8(2) 10(1)	5(3)	0.0434	561.846	117.127	5
2N/O 4Br	1.95(5) 2.36(4)	5(3) 12(2)	neg15(9)	0.1324	1713.597	357.232	5
3N/O 3Br	2.08(3) 2.46(2)	6(2) 13(2)	5(4)	0.0676	874.419	182.289	5
6N/O 1Br	2.08(3) 2.43(2)	11(2) 6(2)	4(3)	0.0762	985.981	205.547	5
1N/O 6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O 2Br	2.08(3) 2.44(2)	10(2) 10(1)	4(3)	0.0506	654.830	136.512	5
2N/O 5Br	1.92(6) 2.34(4)	6(4) 13(2)	neg21(9)	0.1269	1642.697	342.451	5
4N/O 3Br	2.08(3) 2.45(2)	8(2) 13(2)	5(3)	0.0523	676.175	140.962	5
3N/O 4Br	2.09(3) 2.46(2)	6(2) 15(2)	6(4)	0.0772	999.554	208.376	5

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(3)	7(2)					
1S	2.30(5)	7(4)					
1Br	2.43(2)	8(2)	1(3)	0.0171	220.995	79.015	7
2N/O	2.02(3)	5(2)					
2S	2.29(5)	11(4)					
1Br	2.41(2)	7(2)	neg1(4)	0.0172	222.149	79.427	7
1N/O	2.00(3)	2(3)					
3S	2.27(5)	13(3)					
1Br	2.40(2)	7(2)	neg5(5)	0.0185	239.234	85.536	7
2N/O	2.03(2)	3(2)					
1S	2.31(2)	2(2)					
2Br	2.42(3)	15(5)	1(3)	0.0153	198.135	70.842	7
1N/O							
1S							
3Br			No Fit	No Fit	No Fit	No Fit	7
2N/O	2.02(2)	3(2)					
1S	2.29(3)	3(2)					
1Br	2.43(3)	9(4)	0(3)	0.017	219.882	78.617	7
1N/O	1.99(3)	1(2)					
2S	2.27(5)	7(3)					
1Br	2.40(3)	9(4)	neg4(5)	0.0207	267.351	95.589	7
1N/O	2.00(4)	1(2)					
1S	2.27(4)	2(3)					
2Br	2.43(5)	14(6)	neg2(6)	0.0389	503.610	180.062	7

Table G.12. Additional Fits for Zn(II) E63C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(3)	2(2)	12(5)	0.4416	6400.515	381.032	3
3N/O	2.12(3)	4(2)	10(3)	0.3571	5175.240	308.089	3
4N/O	2.12(2)	6(2)	9(3)	0.3280	4753.768	282.999	3
5N/O	2.11(2)	8(2)	8(3)	0.3337	4836.144	287.903	3
6N/O	2.11(3)	10(2)	7(3)	0.3597	5213.359	310.359	3
7N/O	2.10(3)	12(3)	6(3)	0.3973	5759.027	342.843	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.26(2)	6(1)	neg3(5)	0.2882	4177.651	248.702	3
3S	2.25(2)	8(1)	neg5(4)	0.2229	3230.734	192.330	3
4S	2.24(2)	10(1)	neg6(3)	0.2039	2955.021	175.917	3
5S	2.24(2)	12(1)	neg7(3)	0.2094	3034.448	180.645	3
6S	2.23(2)	14(1)	neg8(3)	0.2279	3303.524	196.664	3
7S	2.23(3)	16(2)	neg9(3)	0.2531	3668.899	218.415	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.07(2)	2(2)					
1N/O	2.20(2)	5(1)	9(3)	0.2363	3425.147	231.462	5
2N/O	2.03(2)	1(2)					
2N/O	2.18(2)	2(2)	8(2)	0.2566	3719.200	251.334	5
3N/O	2.07(2)	1(2)					
1N/O	2.20(2)	4(1)	8(2)	0.2386	3458.830	233.739	5
4N/O	2.07(2)	4(2)					
1N/O	2.20(2)	3(2)	7(2)	0.2718	3938.932	266.183	5
3N/O	2.04(2)	2(2)					
2N/O	2.18(2)	1(2)	6(2)	0.2927	4242.205	286.677	5
5N/O	2.06(3)	7(3)					
1N/O	2.19(3)	2(2)	6(3)	0.3199	4637.133	313.365	5
4N/O	2.04(3)	6(3)					
2N/O	2.18(3)	0(3)	5(3)	0.3423	4961.840	335.308	5
3N/O	2.01(4)	4(4)					
3N/O	2.16(3)	2(3)	5(3)	0.3607	5227.897	353.288	5
6N/O	2.06(3)	10(3)					
1N/O	2.18(3)	1(3)	4(3)	0.3718	5388.678	364.153	5
5N/O	2.04(6)	13(8)					
2N/O	2.15(5)	3(5)	4(4)	0.3895	5645.625	381.517	5
4N/O	2.46(2)	2(1)					
3N/O	2.02(3)	6(2)	neg9(4)	0.1482	2147.335	145.111	5

Zn-S(2.2) Zn-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(2)	3(1)					
1S	2.31(2)	1(1)	neg8(3)	0.1332	1929.911	130.418	5

2S	2.14(2)	4(2)					
2S	2.29(2)	2(1)	neg9(3)	0.1462	2119.220	143.211	5
3S	2.18(2)	7(1)					
1S	2.31(2)	0(1)	neg9(3)	0.1412	2047.058	138.335	5
4S	2.26(3)	11(2)					
1S	1.80(7)	23(14)	neg(5)	0.1939	2810.900	189.953	5
3S	2.15(3)	8(2)					
2S	2.29(2)	4(2)	neg10(3)	0.1726	2501.385	169.037	5
5S	2.24(3)	13(1)					
1S	2.60(2)	3(2)	neg9(4)	0.1214	1758.968	118.866	5
4S	2.26(2)	7(2)					
2S	2.11(4)	7(3)	neg10(4)	0.2020	2927.403	197.826	5
3S	2.13(4)	10(4)					
3S	2.27(3)	7(3)	neg11(4)	0.2081	3016.642	203.857	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.24(3)	12(2)					
2S	1.86(0.12)	38(26)	neg5(6)	0.1987	2879.674	194.601	5
4S	2.27(2)	10(1)					
3S	2.62(4)	19(7)	neg2(4)	0.1683	2443.339	165.114	5

Zn-N(2.0) Zn-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.04(2)	1(1)					5
1S	2.30(2)	1(1)	2(3)	0.1388	2012.234	135.982	
1N/O	1.99(2)	1(2)					5
2S	2.28(2)	4(1)	neg2(3)	0.1467	2126.241	143.686	
2N/O	2.00(3)	4(2)					
2S	2.28(2)	5(1)	neg1(3)	0.1610	2334.103	157.733	5
3N/O	2.04(2)	5(2)					
1S	2.31(2)	1(1)	2(3)	0.1500	2174.237	146.929	5
1N/O	1.97(3)	1(2)					
3S	2.27(2)	7(1)	neg4(3)	0.1678	2431.746	164.331	5
1N/O	2.08(0.19)	16(61)					
4S	2.25(3)	11(4)	neg5(6)	0.2005	2906.682	196.426	5

4N/O	2.05(3)	8(2)					
1S	2.30(2)	2(2)	3(3)	0.1764	2556.837	172.784	5
2N/O	2.03(9)	11(9)					
3S	2.26(3)	9(2)	neg2(5)	0.1936	2805.772	189.607	5
3N/O	2.04(6)	10(4)					
2S	2.28(3)	6(2)	0(4)	0.1850	2681.651	181.219	5
5N/O	2.07(5)	13(3)					
1S	2.30(2)	3(2)	4(4)	0.2021	2928.711	197.915	5
1N/O	1.59(0.11)	19(19)					
5S	2.24(2)	12(1)	neg7(4)	0.2007	2908.220	196.530	5
4N/O	2.10(0.10)	15(9)					
2S	2.28(3)	7(3)	3(7)	0.1932	2799.863	189.207	5
2N/O	2.13(0.13)	21(76)					
4S	2.25(3)	11(4)	neg4(8)	0.1993	2889.006	195.231	5
3N/O	2.09(0.10)	17(22)					
3S	2.26(3)	9(4)	neg1(8)	0.1956	2834.761	191.566	5
6N/O	2.10(7)	17(4)					
1S	2.29(2)	4(2)	4(5)	0.2232	3234.710	218.593	5
1N/O	2.20(3)	2(2)					
6S	2.22(2)	11(1)	neg9(3)	0.1749	2535.042	171.312	5
5N/O	2.14(9)	18(13)					
2S	2.28(2)	7(3)	5(8)	0.1965	2848.296	192.480	5
2N/O	2.21(2)	1(1)					
5S	2.22(2)	8(1)	neg8(3)	0.1412	2046.687	138.310	5
4N/O	2.13(0.10)	19(29)					
3S	2.27(3)	9(4)	1(10)	0.1956	2835.621	191.624	5
3N/O	2.15(0.11)	26(82)					
4S	2.25(3)	11(3)	neg3(11)	0.1982	2872.327	194.104	5

Zn-N(2.0) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	2(2)					5
1Br	2.44(2)	5(1)	4(4)	0.1960	2841.041	191.990	
1N/O	1.41(0.17)	13(23)	neg24(12)	0.4366	6327.999	427.630	5

2Br	2.32(4)	8(2)					
2N/O	2.05(3)	3(2)					
2Br	2.43(2)	9(1)	1(5)	0.1970	2855.766	192.985	5
3N/O	2.07(2)	5(1)					
1Br	2.44(2)	5(1)	5(3)	0.1461	2117.801	143.115	5
1N/O	1.95(4)	0(2)					
3Br	2.35(3)	10(1)	neg17(7)	0.2473	3584.597	242.238	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.08(2)	7(2)					
1Br	2.44(1)	6(1)	4(3)	0.1336	1936.750	130.880	5
2N/O	2.03(3)	4(2)					
3Br	2.42(3)	11(1)	neg2(5)	0.2032	2945.259	199.033	5
3N/O	2.06(3)	5(2)					
2Br	2.44(2)	9(1)	3(3)	0.1549	2244.486	151.676	5
5N/O	2.08(2)	9(2)					
1Br	2.44(1)	6(1)	4(3)	0.1431	2074.665	140.200	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.07(2)	8(2)					
2Br	2.44(2)	10(1)	3(3)	0.1420	2057.858	139.065	5
2N/O	2.02(4)	4(2)					
4Br	2.42(3)	13(1)	neg4(6)	0.2113	3062.853	206.980	5
3N/O	2.06(3)	6(2)					
3Br	2.44(2)	12(1)	2(4)	0.1665	2413.099	163.071	5
6N/O	2.07(3)	11(2)					
1Br	2.43(2)	6(1)	3(3)	0.1644	2382.612	161.011	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.07(3)	10(2)					
2Br	2.44(2)	10(1)	3(3)	0.1476	2139.928	144.611	5
2N/O	1.93(4)	6(3)					
5Br	2.34(3)	13(1)	neg20(7)	0.2129	3085.911	208.538	5

4N/O	2.07(3)	8(2)					
3Br	2.44(2)	12(2)	3(3)	0.1532	2220.966	150.087	5
3N/O	2.06(3)	7(2)					
4Br	2.44(2)	13(2)	2(4)	0.1777	2575.344	174.035	5

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.04(3)	6(2)					
1S	2.30(6)	7(6)					
1Br	2.42(2)	7(3)	1(4)	0.1109	1607.086	125.575	7
2N/O	2.02(4)	5(3)					
2S	2.29(6)	12(5)					
1Br	2.41(2)	7(2)	neg2(5)	0.1081	1566.196	122.380	7
1N/O	2.46(2)	3(1)					
3S	2.20(2)	9(1)					
1Br	2.81(8)	15(10)	neg12(4)	0.1100	1593.954	124.549	7
2N/O	2.03(3)	3(2)					
1S	2.31(3)	2(3)					
2Br	2.41(3)	14(6)	0(4)	0.1089	1578.862	123.369	7
1N/O	1.81(0.13)	10(14)					
1S	2.09(4)	3(2)					
3Br	2.34(3)	9(1)	neg25(7)	0.1499	2172.942	169.790	7
2N/O	2.02(3)	3(2)					
1S	2.30(4)	3(3)					
1Br	2.42(3)	9(4)	0(4)	0.1097	1590.348	124.267	7
1N/O	1.99(3)	1(3)					
2S	2.27(5)	8(3)					
1Br	2.40(3)	8(4)	neg4(5)	0.1122	1626.691	127.107	7
1N/O	2.00(3)	1(2)					
1S	2.28(4)	2(3)					
2Br	2.42(4)	14(6)	neg2(5)	0.1315	1906.103	148.939	7

Zn-N(2.0) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(4)	10(4)					
1Imd	2.15(6)	3(5)	5(3)	0.3164	4586.492	309.943	5
4N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

3N/O	1.98(7)	20(14)					
1Imd	2.19(2)	11(2)					
1Imd	2.06(2)	12(2)					
1Imd	1.95(3)	8(2)	1(2)	0.1971	2857.248	264.613	9
2N/O	2.05(6)	7(9)					
1Imd	2.06(4)	13(3)					
1Imd	1.85(8)	0(12)					
1Imd	1.94(5)	10(5)					
1Imd	2.18(3)	11(2)	neg1(3)	0.1918	2779.529	315.933	11
1N/O	2.09(4)	2(4)					
1Imd	2.17(3)	17(3)					
1Imd	1.71(7)	3(12)					
1Imd	1.94(4)	20(4)					
1Imd	2.05(4)	21(4)					
1Imd	1.83(4)	16(6)	neg3(3)	0.1342	1944.711	286.077	13
4N/O	2.08(4)	8(4)					
1Imd	2.16(6)	2(5)	6(3)	0.3039	4404.877	297.670	5
3N/O	2.04(5)	9(6)					
1Imd	2.18(3)	4(3)					
1Imd	2.05(4)	3(3)	4(3)	0.2587	3749.473	292.977	7
2N/O	1.99(8)	14(14)					
1Imd	2.19(2)	20(2)					
1Imd	2.06(3)	11(2)					
1Imd	1.95(3)	8(3)	1(2)	0.1992	2886.930	267.362	9
1N/O	2.08(6)	1(7)					
1Imd	2.19(3)	14(2)					
1Imd	1.96(3)	14(4)					
1Imd	2.07(3)	15(3)					
1Imd	1.85(4)	7(6)	neg1(2)	0.1802	2612.321	296.927	11
0N/O							
1Imd	1.86(4)	13(6)					
1Imd	2.19(3)	6(3)					
1Imd	2.07(3)	19(4)					
1Imd	1.75(0.13)	8(25)					
1Imd	1.96(3)	18(5)	neg2(3)	0.1759	2550.055	289.850	11
3N/O	2.08(4)	6(4)					
1Imd	2.16(6)	2(5)	7(3)	0.3141	4552.323	307.634	5
2N/O	2.04(5)	6(7)					
1Imd	2.18(3)	4(3)					
1Imd	2.05(4)	3(3)	5(3)	0.2752	3988.085	311.621	7

1N/O	2.04(8)	4(10)					
1Imd	1.94(3)	7(2)					
1Imd	2.19(2)	10(2)					
1Imd	2.06(2)	11(2)	2(2)	0.2077	3009.687	278.730	9
0N/O							
1Imd	2.19(2)	14(2)					
1Imd	1.87(3)	10(4)					
1Imd	1.97(2)	16(3)					
1Imd	2.08(2)	17(3)	neg1(2)	0.1964	2847.136	263.676	9
2N/O	2.10(5)	5(6)					
1Imd	2.14(9)	4(9)	9(4)	0.3601	5218.995	352.686	5
1N/O	2.04(8)	4(11)					
1Imd	2.04(4)	3(3)					
1Imd	2.17(4)	4(3)	5(3)	0.3240	4696.328	366.962	7
0N/O							
1Imd	2.06(2)	12(2)					
1Imd	2.18(2)	11(2)					
1Imd	1.94(2)	9(2)	1(2)	0.2478	3591.218	280.611	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	5(3)					
1S	2.30(1)	1(1)					
1Imd	2.06(2)	1(2)	0(2)	0.0813	1178.253	92.066	7
1N/O	1.99(2)	2(2)					
1S	2.29(1)	1(1)					
1Imd	2.06(2)	2(1)					
1Imd	1.90(3)	1(3)	neg(2)	0.0599	867.962	80.383	9
0N/O							
1S	2.28(1)	2(1)					
1Imd	1.93(2)	6(2)					
1Imd	2.18(3)	6(2)					
1Imd	2.05(2)	8(2)	0(2)	0.0648	939.232	86.983	9

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	6(3)					
1S	2.30(1)	1(1)					
1Imd	2.06(2)	0(2)	0(2)	0.0802	1161.735	90.776	7
1N/O	1.99(2)	2(2)					
1S	2.29(1)	0(1)					
1Imd	2.06(2)	2(1)	neg3(2)	0.0579	839.698	77.765	9

1Imd	1.90(3)	1(3)					
0N/O							
1S	2.28(1)	2(1)					
1Imd	2.18(3)	6(2)					
1Imd	2.05(2)	8(2)					
1Imd	1.93(2)	5(2)	0(2)	0.0610	883.692	81.840	9

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	6(3)					
1S	2.30(1)	1(1)					
1Imd	2.05(2)	0(2)	0(2)	0.0795	1152.568	90.060	7
1N/O	1.99(2)	2(2)					
1S	2.29(1)	0(1)					
1Imd	2.06(2)	2(1)					
1Imd	1.90(3)	2(3)	neg3(2)	0.0567	821.673	76.096	9
0N/O							
1S	2.28(1)	2(1)					
1Imd	2.05(2)	8(2)					
1Imd	2.18(3)	6(2)					
1Imd	1.93(2)	5(2)	neg1(2)	0.0585	847.343	78.473	9

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(6)	4(6)					
1S	2.88(0.32)	28(62)					
1Imd	2.15(0.10)	4(10)	9(4)	0.3469	5028.316	392.903	7
1N/O	2.00(8)	4(12)					
1S	2.68(3)	3(3)					
1Imd	2.03(4)	4(3)					
1Imd	2.16(4)	5(3)	2(3)	0.2632	3814.915	353.303	9
0N/O							
1S	3.06(8)	8(10)					
1Imd	1.94(2)	9(2)					
1Imd	2.18(2)	11(2)					
1Imd	2.06(2)	12(2)	2(3)	0.2308	3344.744	309.760	9

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(5)	4(5)					
1S	2.73(7)	8(8)					
1Imd	2.15(7)	2(5)	6(4)	0.3300	4783.091	373.742	7
1N/O	2.00(8)	4(11)	2(3)	0.2664	3861.657	357.632	9

1S	2.68(4)	3(4)					
1Imd	2.03(4)	4(3)					
1Imd	2.16(3)	5(3)					
0N/O							
1S	2.68(4)	5(5)					
1Imd	1.94(2)	8(2)					
1Imd	2.18(2)	10(2)					
1Imd	2.05(2)	12(2)	1(2)	0.2377	3444.915	319.037	9

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.00(5)	12(5)					
1S	2.30(1)	1(1)					
1Imd	2.04(2)	0(2)	0(3)	0.0985	2485.307	194.197	7
2N/O	1.99(3)	4(3)					
1S	2.30(2)	0(1)					
1Imd	2.07(3)	2(2)					
1Imd	2.24(6)	2(6)	2(2)	0.0749	1085.512	100.530	9
1N/O	1.94(2)	1(3)					
1S	2.28(1)	0(1)					
1Imd	2.86(3)	2(2)					
1Imd	2.04(2)	4(2)					
1Imd	2.18(5)	1(5)	1(2)	0.0391	566.905	64.437	11

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.00(5)	13(5)					
1S	2.30(1)	1(1)					
1Imd	2.04(2)	0(2)	neg1(3)	0.0961	1393.504	108.886	7
2N/O	1.99(3)	4(3)					
1S	2.30(2)	0(1)					
1Imd	2.23(6)	2(6)					
1Imd	2.06(3)	2(2)	2(2)	0.0737	1067.648	98.876	9
1N/O	1.98(2)	1(3)					
1S	2.28(1)	0(1)					
1Imd	1.95(5)	0(4)					
1Imd	2.21(4)	3(3)					
1Imd	2.07(3)	5(2)	0(2)	0.0481	696.985	79.222	11

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.00(5)	13(5)					
1S	2.30(1)	1(1)					
1Imd	2.04(2)	0(2)	neg1(3)	0.0946	1370.721	107.106	7

2N/O	1.99(3)	4(3)					
1S	2.30(2)	1(1)					
1Imd	2.23(6)	3(7)					
1Imd	2.06(3)	2(2)	2(2)	0.0730	1058.423	98.022	9
1N/O	1.98(2)	0(3)					
1S	2.28(1)	0(1)					
1Imd	2.07(3)	5(2)					
1Imd	2.21(4)	3(3)					
1Imd	1.95(5)	0(4)	0(2)	0.0466	675.172	76.743	11

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(4)	6(4)					
1S	2.72(5)	7(6)					
1Imd	2.16(5)	2(4)	6(3)	0.2691	3900.411	304.771	7
2N/O	2.02(5)	7(8)					
1S	2.68(3)	3(3)					
1Imd	2.17(3)	5(2)					
1Imd	2.04(4)	4(3)	3(3)	0.2103	3048.223	282.299	9
1N/O	2.05(9)	4(10)					
1S	2.92(0.48)	34(96)					
1Imd	1.94(3)	7(3)					
1Imd	2.19(3)	10(2)					
1Imd	2.06(3)	11(2)	2(3)	0.2025	2935.344	333.643	11

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(4)	6(4)					
1S	2.72(6)	8(7)					
1Imd	2.16(5)	1(4)	6(3)	0.2725	3950.059	308.650	7
2N/O	2.02(5)	7(8)					
1S	2.68(3)	4(3)					
1Imd	2.04(4)	4(3)					
1Imd	2.17(3)	5(2)	3(3)	0.2133	3091.711	286.326	9
1N/O	1.99(0.11)	7(17)					
1S	2.68(5)	6(5)					
1Imd	2.19(3)	10(2)					
1Imd	1.95(4)	7(4)					
1Imd	2.06(3)	11(3)	1(3)	0.1898	2751.239	312.717	11

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	2(3)	neg2(2)	0.0899	1303.568	101.858	7

2S	2.28(1)	5(1)					
1Imd	2.04(2)	0(2)					
0N/O							
2S	2.28(1)	5(1)					
1Imd	1.93(5)	3(6)					
1Imd	2.03(3)	1(3)	neg3(2)	0.0872	1263.712	98.744	7

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(4)	2(3)					
2S	2.28(1)	5(1)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0923	1337.477	104.508	7
0N/O							
2S	2.28(1)	5(1)					
1Imd	1.92(5)	3(6)					
1Imd	2.03(3)	1(3)	neg4(2)	0.0853	1236.094	96.586	7

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(4)	2(4)					
2S	2.28(2)	5(1)					
1Imd	2.04(3)	0(2)	neg3(2)	0.0946	1371.583	107.173	7
0N/O							
2S	2.28(1)	5(1)					
1Imd	2.03(2)	1(3)					
1Imd	1.92(5)	3(6)	neg4(2)	0.0847	1226.992	95.875	7

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(4)	3(4)					
2S	2.28(2)	5(1)					
1Imd	2.03(3)	0(2)	neg3(2)	0.0976	1414.036	110.490	7
0N/O							
2S	2.28(1)	5(1)					
1Imd	2.03(2)	1(3)					
1Imd	1.92(5)	3(5)	neg4(2)	0.0851	1233.917	96.416	7

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.19(3)	4(2)					
2S	2.97(0.19)	29(37)					
1Imd	2.07(3)	2(2)	11(5)	0.4096	5936.802	463.891	7
0N/O							
2S	2.73(7)	13(8)	3(4)	0.4380	6348.477	496.058	7

1Imd	2.15(3)	4(3)					
1Imd	2.02(3)	4(2)					
	Zn-N(2.0) Zn-S(2.2) Zn-Imd						
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.00(0.21)	31(25)					
2S	2.28(2)	5(1)					
1Imd	2.01(2)	1(2)	neg2(4)	0.1075	1557.633	121.711	7
1N/O	1.71(0.15)	25(28)					
2S	2.27(2)	4(1)					
1Imd	1.91(4)	1(5)					
1Imd	2.03(2)	2(3)	neg4(3)	0.0819	1186.981	109.928	9
0N/O							
2S	2.26(1)	6(2)					
1Imd	2.19(2)	6(2)					
1Imd	1.93(2)	4(2)					
1Imd	2.05(2)	7(2)	neg1(2)	0.0620	898.057	83.170	9
	Zn-N(2.0) Zn-S(2.3) Zn-Imd						
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.02(0.23)	33(28)					
2S	2.28(2)	5(1)					
1Imd	2.01(2)	1(2)	neg2(4)	0.1068	1548.537	121.000	7
1N/O	1.94(3)	0(3)					
2S	2.28(2)	5(2)					
1Imd	2.21(6)	2(6)					
1Imd	2.05(3)	2(2)	0(2)	0.0842	1220.706	113.051	9
0N/O							
2S	2.27(1)	7(2)					
1Imd	2.19(2)	6(2)					
1Imd	2.05(2)	7(2)					
1Imd	1.93(2)	4(2)	neg1(2)	0.0614	889.897	82.414	9
	Zn-N(2.0) Zn-S(2.4) Zn-Imd						
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.03(0.24)	35(32)					
2S	2.28(2)	5(1)					
1Imd	2.01(3)	1(2)	neg3(4)	0.1067	1546.617	120.850	7
1N/O	1.68(0.13)	23(24)					
2S	2.27(2)	5(1)					
1Imd	1.91(4)	1(4)					
1Imd	2.02(2)	2(3)	neg5(3)	0.0798	1156.280	107.084	9
0N/O							
2S	2.27(1)	7(2)	neg1(2)	0.0617	894.332	82.825	9

1Imd	2.19(2)	6(2)					
1Imd	2.05(2)	7(2)					
1Imd	1.93(2)	4(2)					

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(6)	5(6)					
2S	2.97(0.65)	60(164)					
1Imd	2.15(9)	3(8)	9(5)	0.3488	5054.959	394.985	7
1N/O	1.68(0.12)	22(22)					
2S	2.27(2)	4(1)					
1Imd	1.90(4)	1(4)					
1Imd	2.02(2)	2(2)	neg5(3)	0.0802	1162.136	107.627	9
0N/O							
2S	2.27(1)	7(2)					
1Imd	2.18(2)	6(2)					
1Imd	2.05(2)	7(2)					
1Imd	1.93(2)	4(2)	neg2(2)	0.0628	909.760	84.254	9

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(4)	4(5)					
2S	2.78(8)	16(10)					
1Imd	2.16(6)	1(5)	7(4)	0.3412	4945.924	386.465	7
1N/O	1.99(7)	2(7)					
2S	2.72(5)	11(6)					
1Imd	2.17(3)	5(3)					
1Imd	2.05(4)	4(3)	3(3)	0.3155	4572.517	423.465	9
0N/O							
2S	3.06(8)	15(12)					
1Imd	2.06(2)	12(2)					
1Imd	2.18(2)	11(2)					
1Imd	1.94(2)	9(2)	2(3)	0.2370	3435.196	318.137	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(9)	6(19)					
1S	2.18(4)	6(14)					
1S	2.31(2)	0(2)					
1Imd	2.05(3)	0(2)	neg2(4)	0.0714	1034.427	95.799	9
0N/O							
1S	2.17(2)	1(2)					
1S	2.31(1)	2(1)					
1Imd	1.93(3)	1(2)	neg4(2)	0.0393	569.307	52.724	9

1Imd	2.06(2)	2(1)					

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	7(2)					
1S	2.07(2)	3(2)					
1S	2.28(2)	1(1)					
1Imd	2.01(3)	2(3)	neg5(3)	0.0704	1020.890	94.546	9
0N/O							
1S	2.17(2)	1(2)					
1S	2.31(1)	2(1)					
1Imd	1.93(3)	1(2)					
1Imd	2.06(2)	2(1)	neg4(2)	0.0411	595.280	55.130	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(2)	0(2)					
1S	2.30(1)	1(1)					
1S	2.67(3)	8(4)					
1Imd	2.07(2)	1(1)	0(2)	0.0525	760.497	70.430	9
0N/O							
1S	2.31(1)	2(1)					
1S	2.18(1)	0(2)					
1Imd	2.07(2)	2(1)					
1Imd	1.93(2)	0(2)	neg4(2)	0.0372	538.761	49.895	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(2)	0(2)					
1S	2.30(1)	1(1)					
1S	2.68(3)	8(4)					
1Imd	2.07(2)	1(1)	0(2)	0.0520	754.042	69.833	9
0N/O							
1S	2.29(2)	1(1)					
1S	2.65(3)	7(4)					
1Imd	1.97(4)	0(5)					
1Imd	2.06(4)	2(3)	neg1(3)	0.0853	1236.039	114.471	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(8)	6(19)					
1S	2.18(4)	7(16)					
1S	2.31(2)	0(2)					
1Imd	2.05(3)	0(2)	neg2(4)	0.0737	1067.971	98.906	9
0N/O			neg4(2)	0.0392	568.669	52.665	9

1S	2.31(1)	2(1)					
1S	2.17(2)	1(2)					
1Imd	1.93(3)	1(2)					
1Imd	2.06(2)	2(1)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(2)	0(2)					
1S	2.30(1)	1(1)					
1S	2.67(3)	8(4)					
1Imd	2.06(2)	1(1)	0(2)	0.0523	758.717	70.266	9
0N/O							
1S	2.30(2)	1(1)					
1S	2.65(3)	6(4)					
1Imd	2.06(3)	2(3)					
1Imd	1.96(4)	0(5)	neg2(3)	0.0801	1160.477	107.473	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(2)	0(2)					
1S	2.30(1)	1(1)					
1S	2.67(3)	9(4)					
1Imd	2.06(2)	1(1)	0(2)	0.0517	749.991	69.457	9
0N/O							
1S	2.30(2)	1(1)					
1S	2.65(3)	7(4)					
1Imd	1.96(4)	0(5)					
1Imd	2.06(3)	2(3)	neg2(3)	0.0808	1171.673	108.510	9

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(3)	1(2)					
1S	2.66(3)	8(4)					
1S	2.30(1)	1(1)					
1Imd	2.06(2)	1(1)	0(2)	0.0542	785.773	72.771	9
0N/O							
1S	2.30(2)	1(1)					
1S	2.65(3)	7(4)					
1Imd	1.96(4)	0(4)					
1Imd	2.06(3)	2(3)	neg2(3)	0.0770	1115.790	103.334	9

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(2)	0(2)					
1S	2.30(1)	1(1)					
1S	2.67(3)	9(4)	0(2)	0.0515	746.903	69.171	9

1Imd	2.06(2)	1(1)					
0N/O							
1S	2.13(4)	4(3)					
1S	2.55(4)	0(2)					
1Imd	1.40(0.16)	14(19)					
1Imd	2.30(0.10)	3(8)	neg29(9)	0.2113	3062.490	283.620	9

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(3)	1(2)					
1S	2.66(3)	9(4)					
1S	2.30(1)	1(1)					
1Imd	2.06(2)	1(1)	0(2)	0.0529	766.045	70.944	9
0N/O							
1S	2.64(3)	7(4)					
1S	2.30(2)	1(1)					
1Imd	2.06(3)	2(3)					
1Imd	1.96(3)	0(4)	neg2(3)	0.0732	1060.328	98.198	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(7)	11(27)					
1S	2.16(7)	5(7)					
1S	2.31(1)	0(1)					
1Imd	2.06(3)	0(2)	neg1(4)	0.0702	1017.386	94.221	9
1N/O	2.25(3)	8(3)					
1S	2.22(7)	6(11)					
1S	2.25(5)	3(4)					
1Imd	2.08(2)	3(2)					
1Imd	1.93(2)	2(3)	neg3(2)	0.0318	460.796	52.376	11
0N/O							
1S	2.17(2)	2(3)					
1S	2.31(1)	1(1)					
1Imd	2.19(3)	3(4)					
1Imd	2.06(2)	6(2)					
1Imd	1.94(2)	2(2)	neg2(2)	0.0303	438.804	49.876	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(7)	11(30)					
1S	2.15(9)	6(8)					
1S	2.31(1)	0(1)					
1Imd	2.06(3)	0(2)	neg1(4)	0.0709	1027.831	95.188	9
1N/O	2.24(3)	8(3)	neg3(2)	0.0325	470.904	53.525	11

1S	2.24(8)	7(10)					
1S	2.25(4)	2(5)					
1Imd	1.93(2)	2(3)					
1Imd	2.08(2)	3(2)					
0N/O							
1S	2.17(2)	3(3)					
1S	2.31(1)	1(1)					
1Imd	2.06(2)	6(2)					
1Imd	1.94(2)	2(2)					
1Imd	2.19(3)	3(4)	neg2(2)	0.0319	461.668	52.475	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	5(2)					
1S	2.30(1)	1(1)					
1S	2.66(2)	8(3)					
1Imd	2.06(2)	0(1)	0(2)	0.0458	663.768	61.472	9
1N/O	1.97(3)	1(3)					
1S	2.30(1)	1(1)					
1S	2.67(3)	7(3)					
1Imd	2.15(9)	6(15)					
1Imd	2.05(4)	1(2)	1(2)	0.0413	598.713	68.052	11
0N/O							
1S	2.28(2)	2(2)					
1S	2.65(4)	9(5)					
1Imd	1.93(2)	5(2)					
1Imd	2.18(3)	5(3)					
1Imd	2.05(2)	8(2)	0(2)	0.0612	887.224	100.845	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	5(2)					
1S	2.30(1)	1(1)					
1S	2.66(2)	8(3)					
1Imd	2.06(2)	0(1)	0(2)	0.0457	661.880	61.297	9
1N/O	1.97(3)	1(3)					
1S	2.29(1)	1(1)					
1S	2.67(3)	7(3)					
1Imd	2.16(8)	5(13)					
1Imd	2.05(3)	1(2)	1(2)	0.0413	598.026	67.974	11
0N/O							
1S	2.28(2)	2(2)					
1S	2.66(4)	10(6)					
1Imd	2.18(3)	5(3)					
1Imd	2.05(2)	8(2)	0(2)	0.0621	900.166	102.317	11

1Imd	1.93(2)	5(2)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(7)	10(29)					
1S	2.16(9)	6(10)					
1S	2.31(2)	0(1)					
1Imd	2.06(3)	0(2)	neg1(4)	0.0717	1038.504	96.177	9
1N/O	2.24(3)	8(3)					
1S	2.24(3)	3(4)					
1S	2.25(7)	8(10)					
1Imd	1.93(2)	3(3)					
1Imd	2.08(2)	4(2)	neg3(2)	0.0327	824.084	93.669	11
0N/O							
1S	2.31(1)	1(1)					
1S	2.17(2)	3(3)					
1Imd	2.18(3)	2(4)					
1Imd	2.05(2)	5(3)					
1Imd	1.93(2)	2(2)	neg2(2)	0.0319	461.967	52.509	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	5(2)					
1S	2.30(1)	1(1)					
1S	2.66(2)	8(3)					
1Imd	2.06(2)	0(1)	0(2)	0.0449	651.263	60.314	9
1N/O	1.97(3)	1(3)					
1S	2.30(1)	1(1)					
1S	2.66(3)	7(4)					
1Imd	2.09(0.16)	11(21)					
1Imd	2.06(3)	0(2)	0(3)	0.0399	578.608	65.767	11
0N/O							
1S	2.29(1)	2(2)					
1S	2.65(4)	9(5)					
1Imd	2.18(3)	5(3)					
1Imd	2.05(2)	8(2)					
1Imd	1.93(2)	5(2)	0(2)	0.0569	825.133	93.788	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	5(2)					
1S	2.30(1)	1(1)					
1S	2.66(2)	8(3)					
1Imd	2.06(2)	0(1)	0(2)	0.0447	647.524	59.968	9

1N/O	1.97(3)	1(3)					
1S	2.30(1)	1(1)					
1S	2.66(3)	8(4)					
1Imd	2.06(3)	0(2)					
1Imd	2.10(0.15)	11(21)	0(3)	0.0399	577.637	65.657	11
0N/O							
1S	2.29(1)	2(2)					
1S	2.65(4)	10(6)					
1Imd	2.18(3)	5(3)					
1Imd	2.05(2)	8(2)					
1Imd	1.93(2)	5(2)	0(2)	0.0576	835.397	94.955	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	6(3)					
1S	2.65(2)	8(3)					
1S	2.31(1)	1(1)					
1Imd	2.06(2)	0(1)	0(2)	0.0446	646.336	59.858	9
1N/O	1.97(3)	2(4)					
1S	2.30(1)	1(1)					
1S	2.66(3)	8(4)					
1Imd	2.06(2)	0(2)					
1Imd	2.07(0.18)	11(18)	0(3)	0.0387	561.354	63.806	11
0N/O							
1S	2.29(1)	2(2)					
1S	2.64(4)	9(5)					
1Imd	1.93(2)	5(2)					
1Imd	2.05(2)	8(2)					
1Imd	2.18(3)	5(3)	0(2)	0.0539	780.945	88.765	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(2)	5(2)					
1S	2.31(1)	1(1)					
1S	2.66(2)	8(3)					
1Imd	2.06(2)	0(1)	0(2)	0.0439	636.500	58.947	9
1N/O	1.97(3)	2(3)					
1S	2.30(1)	1(1)					
1S	2.66(3)	8(4)					
1Imd	2.08(0.17)	11(19)					
1Imd	2.06(2)	0(2)	0(3)	0.0386	559.338	63.577	11
0N/O							
1S	2.29(1)	2(2)					
1S	2.65(4)	10(6)					
1Imd	1.93(2)	5(2)	0(2)	0.0545	789.320	89.717	11

1Imd	2.05(2)	8(2)					
1Imd	2.18(3)	5(3)					
	Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Imd						
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.99(2)	6(3)					
1S	2.65(2)	8(3)					
1S	2.31(1)	1(1)					
1Imd	2.06(2)	0(1)	0(2)	0.0438	635.113	58.818	9
1N/O	1.98(3)	2(4)					
1S	2.65(3)	8(4)					
1S	2.30(1)	1(1)					
1Imd	2.06(2)	0(2)					
1Imd	2.05(0.18)	11(15)	neg1(3)	0.0377	546.111	62.073	11
0N/O							
1S	2.28(1)	2(1)					
1S	1.47(0.13)	53(34)					
1Imd	1.92(2)	6(2)					
1Imd	2.17(3)	6(2)					
1Imd	2.04(2)	8(2)	neg1(2)	0.0500	724.308	82.328	11
	Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd						
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O	1.96(3)	1(3)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0445	1123.991	104.094	9
0N/O							
1S	2.28(3)	5(4)					
1Br	2.41(2)	7(2)					
1Imd	1.95(3)	1(4)					
1Imd	2.06(3)	1(3)	neg3(2)	0.0516	747.716	69.247	9
	Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd						
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O	1.96(3)	1(2)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0442	641.102	59.373	9
0N/O							
1S	2.28(3)	5(3)					
1Br	2.41(2)	7(2)					
1Imd	2.06(3)	1(3)					
1Imd	1.96(3)	1(4)	neg3(2)	0.0524	759.176	70.308	9
	Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd						

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	1(2)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0441	638.580	59.140	9
0N/O							
1S	2.28(3)	5(3)					
1Br	2.42(2)	7(2)					
1Imd	2.06(3)	1(3)					
1Imd	1.96(3)	1(4)	neg3(2)	0.0532	770.893	71.393	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	1(2)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0441	638.565	59.138	9
0N/O							
1S	2.28(3)	5(3)					
1Br	2.42(2)	7(2)					
1Imd	1.96(3)	1(4)					
1Imd	2.06(3)	1(3)	neg3(2)	0.0540	781.952	72.417	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	1(3)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0448	649.734	60.173	9
0N/O							
1S	2.29(3)	5(3)					
1Br	2.41(2)	7(2)					
1Imd	1.95(3)	1(4)					
1Imd	2.06(3)	1(3)	neg3(2)	0.0508	736.176	68.178	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	1(3)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0446	646.160	59.842	9
0N/O							
1S	2.29(3)	5(3)					
1Br	2.41(2)	7(2)					
1Imd	1.95(3)	1(4)	neg3(2)	0.0514	745.552	69.046	9

1Imd	2.06(3)	1(3)					

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	1(3)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0445	645.240	59.756	9
0N/O							
1S	2.29(3)	5(3)					
1Br	2.41(2)	7(2)					
1Imd	1.95(3)	1(4)					
1Imd	2.06(3)	1(3)	neg3(2)	0.0521	754.667	69.890	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.30(3)	3(2)					
1Br	2.41(2)	9(3)					
1Imd	2.05(2)	0(2)	neg1(3)	0.0457	661.915	61.301	9
0N/O							
1S	2.29(3)	5(4)					
1Br	2.41(2)	7(2)					
1Imd	1.95(3)	0(3)					
1Imd	2.06(3)	1(2)	neg3(2)	0.0490	710.617	65.811	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.30(2)	3(2)					
1Br	2.41(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0452	655.693	60.724	9
0N/O							
1S	2.29(3)	5(4)					
1Br	2.41(2)	7(2)					
1Imd	1.95(3)	1(4)					
1Imd	2.06(3)	1(2)	neg3(2)	0.0495	717.260	66.426	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.30(2)	3(2)					
1Br	2.41(2)	9(3)					
1Imd	2.05(2)	0(1)	neg1(2)	0.0449	651.413	60.328	9
0N/O			neg3(2)	0.0500	725.002	67.143	9

1S	2.29(3)	5(3)					
1Br	2.41(2)	7(2)					
1Imd	2.06(3)	1(3)					
1Imd	1.95(3)	1(4)					

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.29(2)	3(2)					
1Br	2.42(2)	9(3)					
1Imd	2.05(2)	0(1)	neg2(2)	0.0448	649.899	60.188	9
0N/O							
1S	2.29(1)	1(1)					
1Br	2.76(2)	9(2)					
1Imd	2.06(2)	3(2)					
1Imd	1.95(3)	1(3)	neg2(2)	0.0607	879.947	81.493	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.30((3)	3(3)					
1Br	2.41(2)	9(3)					
1Imd	2.05(2)	0(2)	neg2(1)	0.0465	674.684	62.483	9
0N/O							
1S	2.29(3)	5(4)					
1Br	2.40(2)	7(2)					
1Imd	2.06(3)	2(2)					
1Imd	1.95(3)	0(3)	neg3(2)	0.0484	701.595	64.975	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.30(2)	3(2)					
1Br	2.41(2)	9(3)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0461	667.975	61.862	9
0N/O							
1S	2.29(3)	5(4)					
1Br	2.41(2)	7(2)					
1Imd	2.06(3)	2(2)					
1Imd	1.95(3)	0(3)	neg3(2)	0.0488	706.699	65.448	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.30(2)	3(2)					
1Br	2.41(2)	9(3)	neg2(3)	0.0458	663.231	61.422	9

1Imd	2.05(2)	0(1)					
0N/O							
1S	2.30(3)	5(4)					
1Br	2.41(2)	7(3)					
1Imd	2.06(3)	1(2)					
1Imd	1.95(3)	0(3)	neg3(2)	0.0492	713.203	66.050	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(6)	2(7)					
1S	2.82(6)	7(7)					
1Br	2.43(2)	5(1)					
1Imd	2.08(6)	1(4)	1(5)	0.1550	2245.940	207.999	9
0N/O							
1S	2.93(9)	13(13)					
1Br	2.42(2)	4(1)					
1Imd	2.09(2)	4(2)					
1Imd	1.97(2)	3(2)	neg2(3)	0.1283	1859.365	172.198	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
1S	2.95(9)	13(13)					
1Br	2.42(2)	4(1)					
1Imd	1.96(2)	3(2)					
1Imd	2.09(2)	4(2)	neg2(3)	0.1197	1735.107	160.690	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	2(3)					
1S	2.30(3)	3(3)					
1Br	2.41(2)	9(3)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0464	671.810	62.217	9
0N/O							
1S	2.30(3)	5(4)					
1Br	2.40(2)	7(3)					
1Imd	2.06(3)	2(2)					
1Imd	1.95(3)	0(3)	neg3(2)	0.0480	695.327	64.395	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.96(3)	2(3)					
1S	2.30(2)	3(2)					
1Br	2.41(2)	9(3)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0460	666.560	61.731	9
0N/O							
1S	2.30(3)	5(4)					
1Br	2.40(2)	7(3)					
1Imd	2.06(3)	2(2)					
1Imd	1.95(3)	0(3)	neg3(2)	0.0484	700.810	64.903	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.13(4)	6(2)					
1S	2.82(5)	7(4)					
1Br	2.77(4)	4(4)					
1Imd	2.00(4)	4(3)	2(5)	0.2831	4103.093	379.992	9
0N/O							
1S	2.93(9)	13(13)					
1Br	2.42(2)	4(1)					
1Imd	2.09(2)	4(2)					
1Imd	1.97(2)	3(2)	neg2(3)	0.1288	1866.837	172.890	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	7(3)					
1S	2.31(3)	5(3)					
1Br	2.41(2)	7(2)					
1Imd	2.05(2)	0(2)	neg1(2)	0.0448	648.863	60.092	9
1N/O	1.96(3)	3(4)					
1S	2.30(3)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(3)	1(3)					
1Imd	2.09(0.13)	9(17)	neg1(2)	0.0324	470.175	53.442	11
0N/O							
1S	2.28(3)	6(4)					
1Br	2.41(2)	8(2)					
1Imd	2.05(2)	6(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.18(3)	4(4)	neg1(2)	0.0372	539.530	61.325	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	7(3)					
1S	2.30(3)	4(3)					
1Br	2.41(2)	8(3)	neg1(2)	0.0448	648.703	60.077	9

1Imd	2.05(2)	0(2)					
1N/O	1.96(3)	3(4)					
1S	2.30(2)	5(4)					
1Br	2.42(2)	8(3)					
1Imd	2.09(0.12)	9(17)					
1Imd	2.05(3)	1(3)	neg1(2)	0.0325	470.375	53.465	11
0N/O							
1S	2.28(3)	6(4)					
1Br	2.41(2)	8(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.05(2)	7(3)					
1Imd	2.18(3)	4(4)	neg1(2)	0.0381	551.866	62.727	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	7(3)					
1S	2.30(3)	4(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	0(2)	neg1(2)	0.0449	650.727	60.265	9
1N/O	1.96(3)	3(4)					
1S	2.29(2)	4(4)					
1Br	2.42(2)	8(3)					
1Imd	2.05(4)	1(3)					
1Imd	2.10(0.12)	9(18)	neg1(2)	0.0326	472.322	53.686	11
0N/O							
1S	2.28(3)	5(3)					
1Br	2.41(2)	8(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.18(3)	4(3)					
1Imd	2.05(2)	7(3)	neg1(2)	0.0388	561.993	63.878	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	7(3)					
1S	2.30(2)	4(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	0(2)	neg1(2)	0.0451	654.201	60.586	9
1N/O	1.95(2)	2(2)					
1S	2.28(1)	1(1)					
1Br	2.82(2)	8(2)					
1Imd	2.18(4)	0(4)					
1Imd	2.05(2)	4(2)	1(2)	0.0290	421.004	47.853	11
0N/O							
1S	2.28(1)	1(1)	neg1(2)	0.0488	707.233	80.387	11

1Br	2.77(3)	11(3)					
1Imd	2.04(2)	8(2)					
1Imd	2.17(3)	5(3)					
1Imd	1.93(2)	5(2)					

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	5(4)					
1Br	2.41(2)	7(2)					
1Imd	2.05(2)	1(2)	neg1(2)	0.0447	648.067	60.018	9
1N/O	1.96(3)	4(5)					
1S	2.30(3)	5(4)					
1Br	2.41(2)	7(3)					
1Imd	2.05(3)	1(4)					
1Imd	2.07(0.13)	9(16)	neg1(2)	0.0321	465.192	52.876	11
0N/O							
1S	2.28(3)	6(4)					
1Br	2.40(2)	8(3)					
1Imd	2.18(3)	4(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.05(2)	7(2)	neg1(2)	0.0357	516.900	58.753	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	4(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	0(2)	neg1(2)	0.0446	647.007	59.920	9
1N/O	1.96(3)	4(5)					
1S	2.30(2)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(3)	1(3)					
1Imd	2.08(0.13)	9(16)	neg1(2)	0.0321	464.559	52.804	11
0N/O							
1S	2.29(3)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.18(3)	4(3)					
1Imd	2.05(2)	7(2)					
1Imd	1.93(2)	4(2)	neg1(2)	0.0363	526.463	59.840	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	4(3)	neg1(2)	0.0447	648.176	60.028	9

1Br	2.41(2)	8(3)					
1Imd	2.05(2)	0(2)					
1N/O	1.96(3)	3(4)					
1S	2.30(2)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(3)	1(3)					
1Imd	2.08(0.12)	9(17)	neg1(2)	0.0321	465.773	52.942	11
0N/O							
1S	2.29(2)	5(4)					
1Br	2.41(2)	9(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.18(3)	4(3)					
1Imd	2.05(2)	7(2)	neg1(2)	0.0369	534.222	60.722	11

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	7(3)					
1S	2.30(3)	4(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	0(2)	neg1(2)	0.0449	650.889	60.279	9
1N/O	1.96(3)	3(4)					
1S	2.30(2)	4(4)					
1Br	2.42(2)	8(3)					
1Imd	2.05(3)	1(3)					
1Imd	2.08(0.12)	9(17)	neg1(2)	0.0324	469.154	53.326	11
0N/O							
1S	2.28(1)	2(1)					
1Br	2.77(3)	11(3)					
1Imd	2.04(2)	8(2)					
1Imd	2.17(3)	5(3)					
1Imd	1.93(2)	5(2)	neg1(2)	0.0451	652.959	74.218	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	5(4)					
1Br	2.40(2)	7(2)					
1Imd	2.05(2)	1(2)	neg1(2)	0.0446	646.220	59.847	9
1N/O	1.96(4)	4(5)					
1S	2.31(3)	6(5)					
1Br	2.41(2)	7(3)					
1Imd	2.06(0.13)	9(15)					
1Imd	2.05(3)	1(4)	neg1(2)	0.0317	460.114	52.298	11
0N/O			neg1(2)	0.0344	498.643	56.678	11

1S	2.29(3)	6(4)					
1Br	2.40(2)	8(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.17(3)	4(3)					
1Imd	2.05(2)	7(2)					

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	5(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	1(2)	neg1(2)	0.0445	644.593	59.696	9
1N/O	1.96(3)	4(5)					
1S	2.30(3)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(3)	1(4)					
1Imd	2.06(0.13)	9(15)	neg1(2)	0.0317	458.946	52.166	11
0N/O							
1S	2.29(3)	5(4)					
1Br	2.40(2)	8(3)					
1Imd	2.17(3)	4(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.05(2)	7(2)	neg1(2)	0.0349	506.332	57.552	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	4(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	0(2)	neg1(2)	0.0445	645.249	59.757	9
1N/O	1.96(3)	4(5)					
1S	2.30(2)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(3)	1(4)					
1Imd	2.07(0.12)	9(16)	neg1(2)	0.0317	459.718	52.253	11
0N/O							
1S	2.29(2)	5(4)					
1Br	2.40(2)	9(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.17(3)	4(3)					
1Imd	2.05(2)	7(2)	neg1(2)	0.0354	512.492	58.252	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)	neg1(2)	0.0447	647.515	59.967	9

1S	2.31(3)	4(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	0(2)					
1N/O	1.95(2)	1(2)					
1S	2.29(1)	1(1)					
1Br	2.81(3)	8(2)					
1Imd	2.17(4)	1(5)					
1Imd	2.05(2)	3(2)	0(2)	0.0304	440.464	50.065	11
0N/O							
1S	2.29(1)	2(1)					
1Br	2.77(3)	11(3)					
1Imd	1.93(2)	5(2)					
1Imd	2.17(3)	5(3)					
1Imd	2.04(2)	8(2)	neg1(2)	0.0427	618.185	70.265	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(4)					
1S	2.31(3)	5(4)					
1Br	2.40(2)	7(2)					
1Imd	2.05(2)	1(2)	neg1(2)	0.0447	647.744	59.988	9
1N/O	1.96(4)	4(5)					
1S	2.31(3)	6(5)					
1Br	2.41(2)	7(3)					
1Imd	2.05(3)	1(4)					
1Imd	2.04(0.12)	8(14)	neg1(2)	0.0317	459.497	52.228	11
0N/O							
1S	2.29(3)	6(4)					
1Br	2.40(2)	8(3)					
1Imd	2.17(3)	4(3)					
1Imd	2.05(2)	7(2)					
1Imd	1.93(2)	4(2)	neg1(2)	0.0336	487.442	55.405	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	5(4)					
1Br	2.41(2)	7(3)					
1Imd	2.05(2)	1(2)	neg1(2)	0.0446	645.744	59.803	9
1N/O	1.96(4)	4(5)					
1S	2.31(3)	5(5)					
1Br	2.41(2)	7(3)					
1Imd	2.05(0.12)	8(15)					
1Imd	2.05(3)	1(4)	neg1(2)	0.0316	458.080	52.067	11

0N/O							
1S	2.29(2)	5(4)					
1Br	2.40(2)	8(3)					
1Imd	2.05(2)	7(2)					
1Imd	2.17(3)	4(3)					
1Imd	1.93(2)	4(2)	neg1(2)	0.0341	493.685	56.114	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(3)					
1S	2.31(3)	4(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	1(2)	neg2(2)	0.0446	646.057	59.832	9
1N/O	1.96(4)	4(5)					
1S	2.31(3)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(3)	1(4)					
1Imd	2.06(0.12)	8(15)	neg1(2)	0.0316	458.668	52.134	11
0N/O							
1S	2.29(2)	5(4)					
1Br	2.40(2)	9(3)					
1Imd	2.17(3)	4(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.05(2)	7(2)	neg1(2)	0.0344	498.612	56.674	11

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(4)	5(4)					
1S	2.83(4)	6(5)					
1Br	2.43(2)	5(1)					
1Imd	2.10(5)	2(3)	3(3)	0.0980	1420.009	131.508	9
1N/O	2.01(8)	6(11)					
1S	2.94(0.12)	16(20)					
1Br	2.43(2)	5(1)					
1Imd	2.11(4)	3(3)					
1Imd	1.99(4)	2(4)	neg1(3)	0.0834	1209.495	137.476	11
0N/O							
1S	2.94(9)	13(13)					
1Br	2.42(2)	5(2)					
1Imd	2.15(3)	7(4)					
1Imd	1.93(3)	6(4)					
1Imd	2.04(3)	8(4)	neg1(3)	0.0903	1309.005	148.787	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2N/O	1.99(3)	8(4)					
1S	2.31(3)	5(4)					
1Br	2.40(2)	7(2)					
1Imd	2.05(2)	1(2)	neg2(2)	0.0448	648.883	60.094	9
1N/O	2.01(7)	6(10)					
1S	2.97(0.12)	17(21)					
1Br	2.42(2)	5(1)					
1Imd	1.99(4)	1(5)					
1Imd	2.11(3)	3(3)	0(3)	0.0755	1093.756	124.321	11
0N/O							
1S	2.96(9)	13(13)					
1Br	2.42(2)	5(2)					
1Imd	2.15(3)	6(4)					
1Imd	1.93(3)	5(4)					
1Imd	2.04(3)	8(4)	neg1(2)	0.0836	1211.402	137.693	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(4)					
1S	2.31(3)	5(4)					
1Br	2.40(2)	7(3)					
1Imd	2.05(2)	1(2)	neg2(2)	0.0446	646.494	59.872	9
1N/O	1.96(4)	4(5)					
1S	2.31(3)	6(5)					
1Br	2.41(2)	7(3)					
1Imd	2.04(0.12)	8(14)					
1Imd	2.05(3)	1(4)	neg1(2)	0.0315	456.635	51.903	11
0N/O							
1S	2.29(2)	5(4)					
1Br	2.40(2)	8(3)					
1Imd	2.05(2)	7(2)					
1Imd	1.93(2)	4(2)					
1Imd	2.17(3)	4(3)	neg1(2)	0.0336	487.370	55.396	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(3)	8(4)					
1S	2.31(3)	5(3)					
1Br	2.41(2)	8(3)					
1Imd	2.05(2)	1(2)	neg2(2)	0.0446	646.412	59.865	9
1N/O	1.96(4)	4(5)					
1S	2.31(3)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(3)	1(4)					
1Imd	2.05(0.12)	8(14)	neg1(2)	0.0315	456.912	51.934	11

0N/O							
1S	2.29(2)	5(4)					
1Br	2.40(2)	9(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.05(2)	7(2)					
1Imd	2.17(3)	4(3)	neg1(2)	0.0339	491.604	55.878	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(4)	2(4)					
1S	2.87(3)	8(3)					
1Br	2.82(4)	4(3)					
1Imd	2.15(4)	3(3)	6(4)	0.2238	3243.443	300.379	9
1N/O	1.96(4)	4(5)					
1S	2.31(2)	5(4)					
1Br	2.41(2)	8(3)					
1Imd	2.05(0.12)	8(15)					
1Imd	2.05(3)	1(4)	neg1(2)	0.0317	459.408	52.218	11
0N/O							
1S	2.29(2)	5(4)					
1Br	2.40(2)	9(3)					
1Imd	2.17(3)	4(3)					
1Imd	1.93(2)	4(2)					
1Imd	2.05(2)	7(2)	neg1(2)	0.0343	496.434	56.427	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	3(3)					
2S	2.30(3)	10(3)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0407	589.629	54.606	9
0N/O							
2S	2.28(2)	13(3)					
1Br	2.41(1)	6(1)					
1Imd	1.96(3)	2(4)					
1Imd	2.07(3)	0(3)	neg3(2)	0.0338	489.348	45.319	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
2S	2.30(3)	10(3)					
1Br	2.40(1)	7(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0403	583.918	54.077	9
0N/O			neg3(2)	0.0340	492.439	45.605	9

2S	2.29(2)	12(3)					
1Br	2.41(1)	6(1)					
1Imd	2.07(3)	0(3)					
1Imd	1.96(3)	2(4)					

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
2S	2.30(3)	10(3)					
1Br	2.40(1)	7(2)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0401	581.452	53.849	9
0N/O							
2S	2.29(2)	12(3)					
1Br	2.41(1)	6(1)					
1Imd	1.96(3)	2(5)					
1Imd	2.07(3)	0(3)	neg3(2)	0.0343	497.854	46.107	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
2S	2.30(2)	9(3)					
1Br	2.40(1)	7(2)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0401	581.428	53.847	9
0N/O							
2S	2.28(1)	5(1)					
1Br	2.75(2)	9(2)					
1Imd	1.96(5)	2(7)					
1Imd	2.04(5)	0(4)	neg3(2)	0.0597	865.580	80.162	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	3(3)					
2S	2.31(3)	11(3)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0415	601.250	55.682	9
0N/O							
2S	2.29(2)	1(3)					
1Br	2.40(1)	6(1)					
1Imd	1.96(3)	1(4)					
1Imd	2.06(3)	1(2)	neg3(2)	0.0326	472.010	43.713	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
2S	2.31(3)	10(3)					
1Br	2.40(1)	6(1)	neg2(2)	0.0410	593.836	54.996	9

1Imd	2.05(2)	0(2)					
0N/O							
2S	2.29(2)	13(3)					
1Br	2.41(1)	6(1)					
1Imd	2.06(3)	0(2)					
1Imd	1.96(3)	2(4)	neg3(2)	0.0326	472.589	43.767	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
2S	2.30(3)	10(3)					
1Br	2.40(1)	7(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0407	589.984	54.639	9
0N/O							
2S	2.29(2)	12(3)					
1Br	2.41(1)	6(1)					
1Imd	2.07(3)	0(3)					
1Imd	1.96(3)	2(4)	neg3(2)	0.0328	476.028	44.085	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(3)	1(2)					
2S	2.28(1)	5(1)					
1Br	2.77(3)	10(3)					
1Imd	2.03(2)	1(1)	neg3(2)	0.0591	856.841	79.353	9
0N/O							
2S	2.28(1)	5(1)					
1Br	2.74(2)	9(2)					
1Imd	2.04(4)	0(4)					
1Imd	1.95(5)	2(7)	neg3(2)	0.0575	833.778	77.217	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(4)	3(4)					
2S	2.31(3)	11(3)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0421	609.643	56.460	9
0N/O							
2S	2.30(2)	13(3)					
1Br	2.40(1)	6(1)					
1Imd	1.95(3)	1(3)					
1Imd	2.06(3)	1(2)	neg3(2)	0.0315	456.871	42.311	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.96(4)	3(3)					
2S	2.31(3)	11(3)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0415	600.912	55.651	9
0N/O							
2S	2.30(2)	13(3)					
1Br	2.40(1)	6(1)					
1Imd	1.96(3)	1(3)					
1Imd	2.06(3)	1(2)	neg3(2)	0.0314	455.672	42.200	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
2S	2.31(3)	11(3)					
1Br	2.40(1)	7(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0411	596.012	55.197	9
0N/O							
2S	2.30(2)	13(3)					
1Br	2.41(1)	6(1)					
1Imd	2.06(3)	0(2)					
1Imd	1.96(3)	1(4)	neg3(2)	0.0316	457.746	42.392	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	3(3)					
2S	2.31(3)	10(3)					
1Br	2.40(1)	7(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0410	594.116	55.022	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(4)	4(4)					
2S	2.31(3)	12(3)					
1Br	2.40(1)	6(1)					
1Imd	2.05(2)	0(2)	neg2(2)	0.0430	622.716	57.670	9
0N/O							
2S	2.30(2)	13(3)					
1Br	2.40(1)	6(1)					
1Imd	2.06(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0310	449.861	41.662	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(4)	4(4)					
2S	2.31(3)	11(3)					
1Br	2.40(1)	6(1)	neg2(2)	0.0423	612.919	56.763	9

1Imd	2.05(2)	0(2)					
0N/O							
2S	2.30(2)	13(3)					
1Br	2.40(1)	6(1)					
1Imd	2.06(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0309	447.385	41.433	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(6)	3(7)					
2S	2.94(0.13)	26(25)					
1Br	2.42(2)	5(1)					
1Imd	2.07(4)	1(3)	0(5)	0.1565	2267.985	210.040	9
0N/O							
2S	2.30(2)	13(3)					
1Br	2.40(1)	6(1)					
1Imd	1.95(3)	1(3)					
1Imd	2.06(3)	1(2)	neg3(2)	0.0309	448.457	41.532	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
2S	2.30(2)	13(3)					
1Br	2.40(1)	6(1)					
1Imd	2.06(3)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0311	451.007	41.768	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
2S	2.95(7)	18(12)					
1Br	2.42(2)	4(1)					
1Imd	1.96(3)	3(2)					
1Imd	2.09(2)	4(2)	neg2(3)	0.1173	1700.255	157.462	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
2S	2.30(2)	13(3)					
1Br	2.40(1)	6(1)					
1Imd	2.06(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0304	440.652	40.809	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
2S	2.30(2)	13(3)	neg3(2)	0.0304	441.095	40.850	9

1Br	2.40(1)	6(1)					
1Imd	2.06(2)	1(2)					
1Imd	1.95(3)	1(3)					

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
2S	2.77(6)	6(8)					
1Br	2.73(5)	3(4)					
1Imd	2.00(3)	4(2)					
1Imd	2.13(3)	5(3)	1(4)	0.3535	5124.095	474.548	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	1(4)					
1S	2.45(8)	6(16)					
1Br	2.43(4)	4(5)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0376	948.529	107.814	11
0N/O							
1S	2.20(3)	5(4)					
1S	2.34(3)	0(3)					
1Br	2.37(4)	7(5)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0274	397.293	45.158	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	2(5)					
1S	2.44(9)	7(19)					
1Br	2.43(4)	5(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0377	546.588	62.127	11
0N/O							
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(5)					
1S	2.43(9)	9(24)					
1Br	2.43(4)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0380	550.250	62.544	11

0N/O							
1S	2.20(3)	5(4)					
1S	2.34(3)	1(3)					
1Br	2.37(4)	8(5)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0271	392.134	44.572	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.42(9)	6(18)					
1S	2.25(5)	2(5)					
1Br	2.43(4)	6(5)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0382	553.570	62.921	11
0N/O							
1S	2.17(2)	4(4)					
1S	2.31(1)	1(1)					
1Br	2.78(4)	12(5)					
1Imd	2.07(2)	2(2)					
1Imd	1.96(4)	2(3)	neg4(2)	0.0296	428.332	48.686	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	1(4)					
1S	2.46(8)	6(17)					
1Br	2.43(4)	4(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0372	539.712	61.346	11
0N/O							
1S	2.20(3)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	7(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg(2)	0.0272	393.809	44.762	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(5)					
1S	2.45(9)	8(20)					
1Br	2.43(4)	5(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0374	541.825	61.586	11
0N/O							
1S	2.20(3)	6(4)					
1S	2.34(3)	1(3)	neg3(2)	0.0270	390.707	44.409	11

1Br	2.37(4)	7(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)					

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(5)					
1S	2.44(9)	10(25)					
1Br	2.43(3)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0376	545.668	62.023	11
0N/O							
1S	2.20(3)	6(4)					
1S	2.34(3)	1(3)					
1Br	2.37(4)	8(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0268	388.338	44.140	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.26(6)	3(5)					
1S	2.43(0.10)	11(29)					
1Br	2.43(3)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0379	549.447	62.452	11
0N/O							
1S	2.17(2)	5(5)					
1S	2.31(1)	0(1)					
1Br	2.78(3)	12(4)					
1Imd	2.07(2)	2(2)					
1Imd	1.96(4)	2(3)	neg4(2)	0.0305	442.535	50.300	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	1(4)					
1S	2.46(8)	7(17)					
1Br	2.43(3)	4(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0369	534.640	60.769	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	6(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0270	391.056	44.449	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(4)					
1S	2.45(9)	8(20)					
1Br	2.43(3)	5(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0371	537.027	61.041	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	7(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0268	388.167	44.121	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(5)					
1S	2.45(9)	10(24)					
1Br	2.43(3)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0373	541.092	61.503	11
0N/O							
1S	2.20(3)	6(4)					
1S	2.34(3)	1(3)					
1Br	2.37(3)	7(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0266	386.125	43.889	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.26(6)	3(5)					
1S	2.44(0.10)	11(27)					
1Br	2.43(3)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0376	545.051	61.953	11
0N/O							
1S	2.34(2)	0(2)					
1S	2.21(2)	4(4)					
1Br	2.36(4)	9(5)					
1Imd	2.07(2)	2(2)					
1Imd	1.95(3)	0(2)	neg3(2)	0.0267	387.090	43.998	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	2(4)	neg2(3)	0.0368	533.528	60.643	11

1S	2.47(8)	8(20)					
1Br	2.44(3)	5(6)					
1Imd	2.04(2)	0(2)					
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(4)	1(4)					
1Br	2.37(4)	6(3)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0266	384.999	43.761	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(5)					
1S	2.46(9)	10(22)					
1Br	2.43(3)	5(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0370	535.861	60.908	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	6(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0264	382.190	43.441	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.26(5)	2(5)					
1S	2.45(0.10)	11(26)					
1Br	2.43(3)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0372	539.805	61.356	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(3)	1(3)					
1Br	2.37(3)	7(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0262	380.150	43.209	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.26(6)	3(5)					
1S	2.44(0.10)	13(29)					
1Br	2.43(3)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0375	543.714	61.801	11

0N/O							
1S	2.28(2)	1(1)					
1S	2.79(7)	8(12)					
1Br	2.75(3)	6(4)					
1Imd	2.06(3)	3(2)					
1Imd	1.95(3)	1(4)	neg2(3)	0.0566	820.236	93.231	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(3)	1(3)					
1S	2.46(8)	4(13)					
1Br	2.43(4)	4(5)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0369	534.172	60.716	11
0N/O							
1S	2.20(2)	5(4)					
1S	2.35(4)	1(3)					
1Br	2.36(4)	6(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0270	391.187	44.464	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	1(4)					
1S	2.45(8)	6(15)					
1Br	2.43(4)	4(5)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0370	536.641	60.997	11
0N/O							
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	2(4)					
1S	2.45(8)	7(18)					
1Br	2.43(4)	5(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0373	540.757	61.465	11
0N/O							
1S	2.20(2)	5(4)					
1S	2.34(3)	1(3)					
1Br	2.37(4)	7(4)	neg3(2)	0.0266	385.071	43.769	11

1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(5)					
1S	2.44(9)	8(20)					
1Br	2.43(4)	6(6)					
1Imd	2.05(2)	0(2)	neg2(3)	0.0376	544.487	61.889	11
0N/O							
1S	2.31(1)	1(2)					
1S	2.18(2)	4(4)					
1Br	2.78(4)	13(5)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	2(2)	neg4(2)	0.0303	438.454	49.836	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(3)	1(3)					
1S	2.46(8)	5(14)					
1Br	2.43(4)	4(5)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0365	528.857	60.112	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	6(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0268	388.042	44.106	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	1(4)					
1S	2.46(8)	6(15)					
1Br	2.43(4)	4(5)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0367	531.521	60.415	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(3)	6(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0266	384.954	43.755	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.95(3)	1(3)					
1S	2.25(4)	2(4)					
1S	2.45(8)	7(18)					
1Br	2.43(4)	5(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0370	535.782	60.899	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(3)	1(3)					
1Br	2.37(4)	7(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0264	382.593	43.487	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(5)	2(4)					
1S	2.45(9)	8(20)					
1Br	2.43(4)	6(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0372	539.641	61.338	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.34(3)	1(3)					
1Br	2.37(3)	7(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0264	381.967	43.416	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	1(4)					
1S	2.47(8)	6(16)					
1Br	2.44(4)	4(6)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0364	528.241	60.042	11
0N/O							
1S	2.29(2)	1(1)					
1S	2.80(7)	9(13)					
1Br	2.75(3)	6(4)					
1Imd	1.95(3)	1(4)					
1Imd	2.05(3)	2(3)	neg3(3)	0.0536	777.034	88.321	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	2(4)					
1S	2.46(8)	7(18)					
1Br	2.44(3)	5(6)	neg2(2)	0.0366	530.766	60.329	11

1Imd	2.04(2)	0(2)					
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	6(3)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0262	379.127	43.093	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	2(4)					
1S	2.46(9)	9(20)					
1Br	2.44(3)	5(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0369	534.802	60.788	11
0N/O							
1S	2.20(2)	6(4)					
1S	2.35(3)	1(3)					
1Br	2.37(4)	7(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0260	376.814	42.830	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.26(5)	2(5)					
1S	2.45(9)	9(23)					
1Br	2.44(3)	6(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0372	538.531	61.212	11
0N/O							
1S	2.29(2)	1(1)					
1S	2.78(8)	9(13)					
1Br	2.75(3)	7(4)					
1Imd	2.06(3)	3(2)					
1Imd	1.95(3)	1(3)	neg3(3)	0.0553	801.058	91.052	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(3)	1(3)					
1S	2.47(7)	4(12)					
1Br	2.43(4)	3(5)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0363	526.096	59.798	11
0N/O							
1S	2.21(2)	6(4)	neg3(2)	0.0266	386.252	43.903	11

1S	2.36(4)	1(3)					
1Br	2.37(4)	6(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)					

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(3)	1(3)					
1S	2.46(8)	5(13)					
1Br	2.43(4)	4(5)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0365	528.813	60.107	11
0N/O							
1S	2.21(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	6(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0264	382.974	43.530	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.45(8)	5(14)					
1S	2.25(4)	1(4)					
1Br	2.43(4)	5(5)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0375	544.090	61.844	11
0N/O							
1S	2.21(2)	6(4)					
1S	2.35(3)	1(3)					
1Br	2.37(4)	7(4)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(3)	1(3)	neg3(2)	0.0262	380.416	43.240	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.29(2)	1(1)					
1S	2.77(8)	10(13)					
1Br	2.75(3)	7(4)					
1Imd	2.06(3)	3(2)					
1Imd	1.95(3)	1(3)	neg3(3)	0.0542	785.543	89.288	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(3)	1(3)					
1S	2.47(8)	5(14)					
1Br	2.44(4)	4(6)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0363	525.752	59.759	11
0N/O							
1S	2.21(2)	6(4)					
1S	2.36(4)	1(3)					
1Br	2.37(4)	5(3)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(2)	1(2)	neg3(2)	0.0262	380.314	43.228	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	1(4)					
1S	2.46(8)	6(15)					
1Br	2.44(4)	4(6)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0364	528.292	60.048	11
0N/O							
1S	2.21(2)	6(4)					
1S	2.36(4)	1(3)					
1Br	2.37(4)	6(3)					
1Imd	1.95(2)	1(3)					
1Imd	2.07(2)	1(2)	neg3(2)	0.0260	377.201	42.874	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(4)	2(4)					
1S	2.46(8)	7(18)					
1Br	2.44(4)	5(6)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0367	532.295	60.503	11
0N/O							
1S							
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)	neg2(3)	0.0370	535.785	60.899	11

1S	2.26(4)	2(4)					
1S	2.45(9)	8(20)					
1Br	2.44(4)	5(6)					
1Imd	2.04(2)	0(2)					
0N/O							
1S	2.29(2)	1(1)					
1S	2.78(8)	10(13)					
1Br	2.75(3)	7(4)					
1Imd	1.95(3)	1(3)					
1Imd	2.06(3)	3(2)	neg3(3)	0.0542	785.606	89.295	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.21(2)	5(4)					
1S	2.36(4)	1(3)					
1Br	2.37(4)	5(3)					
1Imd	1.95(2)	0(2)					
1Imd	2.07(2)	1(2)	neg4(2)	0.0264	382.641	43.493	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.25(3)	1(4)					
1S	2.46(8)	5(14)					
1Br	2.44(4)	4(6)					
1Imd	2.04(2)	0(2)	neg2(2)	0.0368	533.909	60.686	11
0N/O							
1S	2.21(2)	5(4)					
1S	2.36(4)	1(3)					
1Br	2.37(4)	6(3)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(2)	1(2)	neg4(2)	0.0262	379.294	43.112	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	1(3)					
1S	2.26(4)	2(4)					
1S	2.46(8)	6(16)					
1Br	2.44(4)	5(6)					
1Imd	2.04(2)	0(2)	neg2(3)	0.0371	537.623	61.108	11

0N/O							
1S	2.21(2)	6(4)					
1S	2.35(4)	1(3)					
1Br	2.37(4)	6(3)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(2)	1(2)	neg4(2)	0.0260	376.664	42.813	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
1S	2.94(6)	11(8)					
1S	2.29(3)	5(4)					
1Br	2.41(2)	7(2)					
1Imd	2.06(3)	2(2)					
1Imd	1.94(3)	0(3)	neg4(3)	0.0420	608.838	69.203	11

Table F13. Additional Fits for Ni(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaCl and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	10(1)	5(4)	0.2732	5494.488	327.095	3
3N/O	2.07(1)	3(1)	5(2)	0.1788	3596.559	214.108	3
4N/O	2.08(1)	5(1)	4(2)	0.1401	2817.942	167.756	3
5N/O	2.08(1)	7(1)	4(2)	0.1354	2722.610	162.081	3
6N/O	2.08(1)	9(1)	3(2)	0.1510	3035.995	180.737	3
7N/O	2.08(2)	11(1)	3(2)	0.1778	3575.075	212.829	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(2)	5(1)	neg17(6)	0.2975	5983.760	356.222	3
3S	2.17(2)	8(1)	neg17(5)	0.2513	5053.699	300.854	3
4S	2.17(2)	11(1)	neg17(4)	0.2377	4780.260	284.576	3
5S	2.18(3)	13(1)	neg17(4)	0.2385	4796.296	285.530	3
6S	2.18(3)	15(2)	neg17(4)	0.2456	4940.403	294.109	3
7S	2.18(3)	17(2)	neg17(4)	0.2554	5137.486	305.842	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar

2N/O	2.03(2)	1(2)					
1N/O	2.16(2)	3(2)	4(2)	0.1482	2979.785	201.366	5
2N/O	2.03(3)	2(3)					
2N/O	2.14(3)	2(4)	4(2)	0.1316	2646.506	178.844	5
3N/O	2.05(2)	2(2)					
1N/O	2.17(4)	0(4)	4(2)	0.1320	2654.462	179.382	5
4N/O	2.08(2)	5(1)					
1N/O	2.30(9)	11(15)	6(2)	0.1217	2446.847	165.351	5
3N/O	2.07(1)	3(1)					
2N/O	2.21(9)	17(14)	6(2)	0.1237	2486.830	168.053	5
5N/O	2.09(1)	7(1)					
1N/O	2.37(5)	6(6)	6(2)	0.1143	2298.130	155.302	5
4N/O	2.08(1)	5(1)					
2N/O	2.32(6)	14(10)	7(2)	0.1117	2246.329	151.801	5
3N/O	2.08(1)	3(1)					
3N/O	2.25(7)	22(120	7(2)	0.1167	2347.532	158.640	5
6N/O	2.09(1)	9(1)					
1N/O	2.39(4)	3(4)	6(2)	0.1196	2404.888	162.516	5
5N/O	2.09(1)	6(1)					
2N/O	2.37(4)	10(6)	7(1)	0.1079	2170.971	146.708	5
4N/O	2.09(1)	5(1)					
3N/O	2.33(5)	18(8)	8(2)	0.1086	2185.088	147.663	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.15(3)	5(3)					
1S	2.29(7)	5(7)	neg14(6)	0.2398	4822.496	325.892	5
2S	2.17(2)	5(2)					
2S	2.31(6)	12(8)	neg11(5)	0.2114	4251.883	287.331	5
3S	2.18(3)	7(2)					
1S	2.37(6)	7(7)	neg12(5)	0.2134	4292.269	290.060	5
4S	2.20(3)	9(1)					
1S	2.42(4)	6(5)	neg11(4)	0.1934	3889.767	262.860	5
3S	2.19(2)	7(1)					
2S	2.38(5)	11(6)	neg10(4)	0.1860	3741.517	252.842	5

5S	2.17(3)	12(2)					
1S	1.43(0.18)	33(40)	neg18(5)	0.2333	4692.873	317.132	5
4S	2.21(2)	9(1)					
2S	2.42(4)	10(4)	neg9(3)	0.1665	3348.563	226.287	5
3S	2.38(4)	14(5)					
3S	2.19(2)	7(2)	neg9(4)	0.1781	3582.848	242.119	5
6S	2.14(3)	12(2)					
1S	1.90(4)	9(5)	neg22(5)	0.2206	4435.632	299.748	5
5S	2.22(2)	11(1)					
2S	2.45(3)	8(3)	neg9(3)	0.1535	3086.167	208.555	5
4S	2.21(2)	9(1)					
3S	2.43(3)	12(3)	neg8(3)	0.1450	2915.267	197.006	5

Ni-N(2.0) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.03(3)	2(2)					5
1S	2.27(5)	6(4)	neg2(5)	0.2322	4669.902	315.580	
1N/O	1.99(4)	1(3)					5
2S	2.22(4)	7(3)	neg9(6)	0.2541	5109.847	345.310	
2N/O	2.07(2)	1(1)					
2S	2.50(9)	24(13)	5(3)	0.1995	4012.759	271.172	5
3N/O	2.08(1)	3(1)					
1S	2.58(4)	10(5)	6(2)	0.1297	2608.297	176.262	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O	1.75(5)	7(7)					
4S	2.16(2)	10(1)	neg20(4)	0.2192	4409.197	297.962	5
4N/O	2.08(1)	5(1)					
1S	2.59(3)	9(4)	6(1)	0.0862	1732.886	117.104	5
2N/O	4.14(0.12)	3(12)					
3S	2.17(2)	8(1)	neg16(5)	0.2410	4847.641	327.591	5
3N/O	2.08(1)	3(1)					
2S	2.57(4)	19(6)	6(2)	0.1139	2290.289	154.772	5
5N/O	2.08(2)	7(1)	5(2)	0.1291	2595.962	175.428	5

1S	1.94(0.10)	29(29)					
1N/O	2.29(5)	1(4)					
5S	2.20(3)	12(2)	neg15(5)	0.2246	4517.055	305.251	5
4N/O	2.08(1)	5(1)					
2S	2.59(3)	16(4)	6(1)	0.0761	1530.630	103.436	5
2N/O	2.68(4)	5(4)					
4S	2.19(2)	11(1)	neg13(3)	0.1761	3540.753	239.275	5
3N/O	1.82(0.10)	20(17)					
3S	2.17(3)	8(2)	neg19(6)	0.2266	4557.384	307.976	5
6N/O	2.07(3)	7(2)					
1S	2.00(0.11)	15(13)	4(2)	0.1307	2628.715	177.642	5
1N/O	3.17(0.10)	3(10)					
6S	2.18(3)	15(2)	neg17(4)	0.2211	4445.891	300.442	5
5N/O	2.08(1)	7(1)					
2S	1.95(6)	34(18)	6(2)	0.1237	2488.387	168.159	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.83(0.11)	24(18)					
3S	2.17(3)	8(2)	neg19(7)	0.2248	4522.085	305.591	5
3N/O	3.18(6)	6(6)					
4S	2.17(2)	10(1)	neg17(4)	0.1787	3593.976	242.871	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(2)	7(2)					
1Imd	1.97(8)	11(11)	2(2)	0.1218	2356.722	159.261	5
4N/O	2.08(2)	6(2)					
1Imd	1.90(6)	8(12)					
1Imd	2.04(6)	5(9)	1(2)	0.1043	2098.271	163.955	7
3N/O	2.07(2)	3(2)					
1Imd	1.98(3)	3(4)					
1Imd	1.85(4)	2(5)					
1Imd	2.12(4)	1(4)	0(2)	0.0965	1940.163	179.680	9
2N/O	2.07(2)	1(2)					
1Imd	2.21(0.29)	8(48)					
1Imd	2.12(0.11)	3(12)	2(4)	0.1063	2138.796	243.104	11

1Imd	1.87(0.10)	1(10)					
1Imd	1.99(9)	4(10)					
1N/O	2.08(3)	3(3)					
1Imd	2.37(8)	8(9)					
1Imd	2.24(6)	16(5)					
1Imd	2.01(5)	16(5)					
1Imd	2.12(6)	18(5)					
1Imd	1.90(5)	9(5)	5(3)	0.1128	2267.669	333.586	13
4N/O	2.08(2)	6(2)					
1Imd	2.02(6)	7(7)	3(2)	0.1114	2240.241	151.390	5
3N/O	2.08(2)	4(2)					
1Imd	2.10(0.12)	8(18)					
1Imd	1.97(9)	6(10)	3(3)	0.1079	2170.711	169.615	7
2N/O	2.07(2)	1(2)					
1Imd	2.15(4)	2(4)					
1Imd	2.01(4)	3(4)					
1Imd	1.89(6)	2(7)	2(2)	0.1103	2218.211	205.431	9
1N/O	2.07(3)	2(3)					
1Imd	2.20(4)	9(4)					
1Imd	1.96(4)	11(4)					
1Imd	1.85(4)	5(5)					
1Imd	2.08(4)	12(4)	1(3)	0.1335	2684.105	305.086	11
0N/O							
1Imd	1.88(6)	9(8)					
1Imd	1.98(6)	15(8)					
1Imd	2.20(8)	13(12)					
1Imd	2.28(0.20)	1(40)					
1Imd	2.09(6)	16(9)	4(3)	0.2463	4953.895	563.080	11
3N/O	2.09(2)	4(2)					
1Imd	2.03(6)	5(6)	4(2)	0.1225	2464.494	166.544	5
2N/O	2.08(2)	1(2)					
1Imd	2.15(4)	1(4)					
1Imd	1.99(3)	1(3)	4(2)	0.1240	2494.573	194.921	7
1N/O	2.07(2)	2(2)					
1Imd	2.17(4)	4(4)					
1Imd	2.04(6)	3(7)					
1Imd	1.94(7)	0(11)	3(3)	0.1489	2995.272	277.395	9
0N/O							
1Imd	2.21(4)	10(5)					
1Imd	1.99(3)	13(4)	3(2)	0.2579	5186.616	480.338	9

1Imd	1.88(4)	7(5)					
1Imd	2.10(3)	14(4)					
2N/O	2.08(3)	2(2)					
1Imd	2.04(6)	4(5)	4(3)	0.1713	3445.923	232.866	5
1N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7
0N/O							
1Imd	2.06(7)	5(13)					
1Imd	2.17(6)	4(9)					
1Imd	1.97(9)	2(15)	4(3)	0.2950	5932.920	463.587	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.58(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0553	1112.935	86.963	7
3N/O	2.09(1)	4(2)					
1S	2.59(3)	8(3)					
1Imd	2.18(4)	3(4)					
1Imd	2.01(3)	2(3)	6(1)	0.0514	1033.334	95.698	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	2.21(6)	0(10)					
1Imd	2.08(8)	1(16)					
1Imd	1.97(8)	1(10)	5(2)	0.0617	1240.148	140.960	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.59(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0531	1068.314	83.476	7
3N/O	2.09(1)	4(2)					
1S	2.59(2)	8(3)					
1Imd	2.18(4)	4(4)					
1Imd	2.01(3)	3(3)	5(1)	0.0493	991.415	91.816	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	2.20(6)	0(9)					
1Imd	1.97(0.10)	2(13)					
1Imd	2.07(9)	0(18)	5(2)	0.0588	1183.547	134.527	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.59(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0515	1035.399	80.904	7
3N/O	2.09(1)	4(2)					
1S	2.59(2)	8(3)					
1Imd	2.01(3)	3(3)					
1Imd	2.17(4)	4(4)	5(1)	0.0479	963.906	89.268	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	1.96(0.11)	2(15)					
1Imd	2.20(5)	0(8)					
1Imd	2.07(9)	0(17)	5(2)	0.057	1145.370	130.188	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.60(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0502	1010.598	78.966	7
3N/O	2.08(1)	4(2)					
1S	2.59(2)	8(3)					
1Imd	2.17(4)	4(4)					
1Imd	2.01(3)	3(3)	5(1)	0.0469	944.130	87.437	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	2.06(9)	0(15)					
1Imd	2.19(5)	1(7)					
1Imd	1.96(0.11)	3(15)	4(2)	0.0555	1115.911	126.839	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.60(2)	9(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0493	991.533	77.477	7
3N/O	2.08(1)	4(2)					
1S	2.60(2)	8(3)					
1Imd	2.01(3)	3(3)					
1Imd	2.17(4)	4(4)	5(1)	0.0461	926.610	85.814	9

2N/O	2.08(2)	1(2)					
1S	2.58(4)	9(4)					
1Imd	2.05(8)	0(13)					
1Imd	1.96(0.10)	3(15)					
1Imd	2.19(4)	1(6)	4(2)	0.0542	1089.150	123.797	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	5(2)					
2S	2.58(3)	16(4)					
1Imd	2.08(4)	6(5)	6(1)	0.0604	1214.643	94.910	7
2N/O	2.08(1)	1(1)					
2S	2.58(3)	15(4)					
1Imd	2.17(2)	1(2)					
1Imd	2.01(2)	0(2)	6(1)	0.0549	1103.446	102.191	9
1N/O	2.07(2)	2(2)					
2S	2.54(6)	17(6)					
1Imd	2.05(5)	5(6)					
1Imd	1.94(5)	1(7)					
1Imd	2.18(4)	5(4)	4(2)	0.083	1669.293	189.739	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.59(3)	16(4)					
1Imd	2.08(4)	6(5)	6(1)	0.058	1167.253	91.207	7
2N/O	2.08(1)	1(1)					
2S	2.58(3)	15(4)					
1Imd	2.01(2)	0(2)					
1Imd	2.17(2)	0(2)	6(10	0.0529	1064.611	98.595	9
1N/O	2.07(2)	2(2)					
2S	2.54(5)	17(6)					
1Imd	2.17(3)	5(4)					
1Imd	1.94(5)	1(7)					
1Imd	2.05(4)	5(5)	4(2)	0.0795	1599.147	181.766	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.59(3)	16(4)					
1Imd	2.07(4)	6(5)	6(1)	0.0567	1140.063	89.082	7

2N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.59(3)	17(4)					
1Imd	2.07(4)	6(5)	5(1)	0.056	1126.948	88.058	7
2N/O	2.08(1)	1(1)					
2S	2.59(3)	16(4)					
1Imd	2.16(2)	0(2)					
1Imd	2.00(2)	0(2)	5(1)	0.0523	1051.269	97.359	9
1N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.60(3)	17(4)					
1Imd	2.07(4)	6(5)	5(1)	0.0556	1117.943	87.354	7
2N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.06(2)	2(2)					
2S	2.54(5)	19(6)					
1Imd	2.04(4)	5(4)					
1Imd	2.17(3)	5(3)					
1Imd	1.93(4)	1(6)	3(2)	0.0743	1495.056	169.934	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.62(3)	5(3)					
1S	2.45(5)	11(6)					
1Imd	2.05(5)	6(5)	5(1)	0.0469	87.309	942.749	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	6(4)					
1S	2.60(3)	3(2)					
1Imd	2.13(3)	0(2)					
1Imd	1.97(3)	0(2)	4(2)	0.0341	77.960	685.881	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.89(7)	6(12)					
1Imd	1.95(4)	4(3)	1(2)	0.0331	98.013	666.275	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.43(6)	12(7)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.045	905.017	83.815	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	6(4)					
1S	2.60(3)	3(2)					
1Imd	2.13(3)	1(2)					
1Imd	1.97(3)	0(2)	4(2)	0.0341	686.000	77.974	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	1.95(4)	4(3)					
1Imd	1.89(6)	5(10)					
1Imd	2.11(3)	4(2)	0(2)	0.0313	628.650	92.478	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.42(6)	13(7)					
1S	2.619(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0445	894.140	82.807	9
2N/O	2.07(1)	0(1)	3(2)	0.0339	681.773	77.493	11

1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.13(3)	1(2)					
1N/O	2.04(2)	6(2)					
1S	2.34(3)	0(3)					
1S	2.55(3)	1(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.88(6)	5(10)					
1Imd	1.95(4)	4(2)	0(2)	0.0294	592.244	87.122	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.42(6)	13(8)					
1S	2.61(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.044	884.804	81.943	9
2N/O	2.07(1)	0(1)					
1S	2.39(4)	7(5)					
1S	2.60(3)	4(2)					
1Imd	2.12(3)	1(3)					
1Imd	1.96(3)	0(2)	3(2)	0.0336	675.221	76.748	11
1N/O	2.04(2)	6(2)					
1S	2.34(3)	0(3)					
1S	2.55(3)	1(2)					
1Imd	1.88(6)	5(9)					
1Imd	1.95(4)	4(2)					
1Imd	2.11(3)	4(2)	0(2)	0.0279	561.056	82.534	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.62(3)	5(3)					
1S	2.45(5)	12(7)					
1Imd	2.05(5)	6(5)	5(1)	0.0454	913.046	84.558	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	6(4)					
1S	2.60(3)	3(2)					
1Imd	2.13(3)	0(2)					
1Imd	1.96(3)	0(2)	3(2)	0.0335	673.515	76.554	11
1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)	0(2)	0.0308	620.411	91.266	11

1Imd	1.89(6)	5(11)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(4)	4(2)					

Ni-N(2.2) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	0(1)					
1S	2.61(3)	2(2)					
1S	2.43(4)	6(4)					
1Imd	1.97(2)	0(2)					
1Imd	2.13(3)	0(2)	3(1)	0.0317	637.618	72.474	11
1N/O	2.05(2)	6(2)					
1S	2.56(3)	1(3)					
1S	2.37(3)	0(4)					
1Imd	1.95(4)	5(3)					
1Imd	2.11(3)	4(2)					
1Imd	1.89(7)	5(10)	0(2)	0.0343	688.909	101.342	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.43(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0443	890.838	82.501	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.0333	669.891	76.143	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.89(6)	5(10)					
1Imd	1.95(4)	4(2)	0(2)	0.029	583.969	85.905	11

Ni-N(2.2) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.42(4)	7(5)					
1S	2.61(3)	3(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.13(3)	1(3)	3(1)	0.0327	658.585	74.857	11

1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	1.87(6)	5(8)					
1Imd	1.95(3)	5(2)					
1Imd	2.10(3)	4(2)	0(2)	0.031	624.037	91.799	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.42(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0439	882.159	81.698	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.033	664.144	75.489	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.88(6)	5(10)					
1Imd	1.95(3)	4(2)	0(2)	0.0275	552.635	81.295	11

Ni-N(2.2) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(1)	1(1)					
1S	2.41(4)	8(5)					
1S	2.61(3)	4(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.12(3)	1(3)	3(1)	0.0325	654.174	74.356	11
1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.56(3)	1(2)					
1Imd	2.10(3)	4(2)					
1Imd	1.87(5)	5(8)					
1Imd	1.95(3)	5(2)	0(2)	0.0293	589.901	86.778	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)	4(1)	0.0439	882.159	81.698	9

1S	2.42(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)					
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.033	664.144	75.489	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.88(6)	5(10)					
1Imd	1.95(3)	4(2)	0(2)	0.0275	552.635	81.295	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.44(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0442	889.665	82.393	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	7(4)					
1S	2.60(3)	3(2)					
1Imd	2.12(3)	1(2)					
1Imd	1.96(3)	0(2)	3(2)	0.033	663.253	75.388	11
2N/O	2.08(1)	1(2)					
1S	2.42(4)	8(5)					
1S	2.61(3)	4(3)					
1Imd 0°	2.12(3)	1(3)					
1Imd 5°	1.97(3)	0(2)	4(1)	0.0338	680.355	77.332	11
2N/O	2.06(3)	3(3)					
1S	2.39(5)	10(7)					
1S	2.59(3)	5(3)					
1Imd 0°	2.02(8)	9(8)					
1Imd 10°	2.08(5)	3(6)	3(2)	0.0384	771.888	87.736	11
2N/O	2.06(3)	3(3)					
1S	2.39(5)	10(7)					
1S	2.59(3)	5(3)					
1Imd 5°	2.02(9)	8(8)					
1Imd 10°	2.09(5)	3(5)	3(2)	0.0394	791.951	90.016	11
1N/O	2.05(2)	6(2)	0(2)	0.029	583.773	85.876	13

1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	1.89(6)	5(10)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(4)	4(2)					

Ni-N(2.2) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.42(4)	7(5)					
1S	2.61(3)	3(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.12(3)	1(3)	3(1)	0.0322	646.809	73.519	11
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	1.95(3)	5(2)					
1Imd	1.88(6)	5(8)					
1Imd	2.11(3)	4(2)	0(2)	0.0309	622.370	91.554	11

Ni-N(2.2) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	6(3)					
1N/O	2.16(5)	5(5)					
1S	2.39(0.14)	18(27)					
1S	2.57(6)	6(7)					
1Imd	1.93(4)	1(4)					
1Imd	2.10(4)	2(4)	3(2)	0.0303	609.696	89.690	13

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.43(6)	14(8)					
1S	2.62(3)	6(3)					
1Imd	2.04(5)	6(5)	4(1)	0.0438	881.627	81.648	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.0327	658.034	74.795	11
2N/O	2.08(1)	1(2)					
1S	2.42(5)	9(5)					
1S	2.61(3)	4(3)					
1Imd 0°	2.12(3)	1(3)	4(2)	0.0338	680.523	77.351	11

1Imd 5°	1.97(3)	0(2)					
2N/O	2.06(3)	3(3)					
1S	2.38(5)	9(6)					
1S	2.59(3)	5(3)					
1Imd 0°	2.01(8)	9(7)					
1Imd 10°	2.08(5)	3(6)	3(2)	0.0377	757.520	86.103	11
2N/O	2.06(3)	3(3)					
1S	2.39(5)	10(7)					
1S	2.59(3)	5(3)					
1Imd 5°	2.01(9)	8(8)					
1Imd 10°	2.09(5)	3(5)	3(2)	0.0389	781.398	88.817	11
1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(3)	4(2)					
1Imd	1.88(6)	5(10)	0(2)	0.0274	551.623	81.147	13

Ni-N(2.2) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(1)	1(1)					
1S	2.42(4)	8(5)					
1S	2.61(3)	4(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.12(3)	1(3)	3(1)	0.032	643.399	73.131	11
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	1.87(5)	5(8)					
1Imd	2.10(3)	4(2)					
1Imd	1.95(3)	5(2)	0(2)	0.0292	587.576	86.435	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	6(2)					
1N/O	1.94(7)	11(12)					
1S	2.38(3)	0(3)					
1S	2.58(3)	1(2)					
1Imd	1.95(2)	5(2)					
1Imd	2.11(2)	3(2)	1(2)	0.0235	472.054	69.442	13
1N/O	2.11(3)	5(3)					
1N/O	1.99(3)	4(3)					
1S	2.40(5)	5(6)					
1S	2.60(4)	3(4)	2(2)	0.0326	654.856	96.333	13

1Imd 0°	1.97(7)	7(7)					
1Imd 10°	2.10(6)	3(6)					

Ni-N(2.0) Ni-Cl(2.4) Ni-Cl(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	4(2)					
1Cl	2.39(5)	13(7)					
1Cl	2.59(3)	6(3)					
1Imd	2.04(5)	6(5)	4(2)	0.0451	906.107	83.915	9
2N/O	2.06(1)	0(1)					
1Cl	2.37(4)	6(4)					
1Cl	2.57(3)	4(2)					
1Imd	2.11(3)	1(3)					
1Imd	1.95(3)	0(2)	2(2)	0.033	663.374	75.402	11
1N/O	2.04(2)	6(2)					
1Cl	2.32(3)	0(3)					
1Cl	2.53(3)	1(2)					
1Imd	1.88(5)	5(10)					
1Imd	1.95(4)	4(2)					
1Imd	2.10(3)	4(2)	0(2)	0.0255	513.237	75.500	11

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.62(3)	5(3)					
1S	2.45(6)	13(8)					
1Imd	2.05(5)	6(5)	4(1)	0.0444	893.875	82.783	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	2.12(3)	1(2)					
1Imd	1.96(3)	0(2)	3(2)	0.0327	656.759	74.650	11
2N/O	2.09(2)	3(2)					
1S	1.82(8)	35(13)					
1S	2.61(2)	9(3)					
1Imd 0°	2.17(3)	2(3)					
1Imd 5°	2.02(3)	1(3)	6(1)	0.0336	675.360	76.764	11
2N/O	2.06(3)	3(3)					
1S	2.59(3)	4(3)					
1S	2.39(5)	10(7)					
1Imd 0°	2.01(8)	8(7)					
1Imd 10°	2.08(5)	3(6)	3(2)	0.0391	785.484	89.281	11
2N/O	2.06(3)	3(3)	3(2)	0.04	803.726	91.355	11

1S	2.60(3)	4(3)					
1S	2.40(5)	10(7)					
1Imd 5°	2.02(8)	8(7)					
1Imd 10°	2.09(5)	3(5)					
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(3)	4(2)					
1Imd	1.88(6)	5(9)	0(2)	0.0276	554.494	81.569	13

Ni-N(2.2) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.42(4)	7(5)					
1S	2.61(3)	3(2)					
1Imd	2.12(3)	1(3)					
1Imd	1.97(3)	0(2)	3(1)	0.0317	636.960	72.399	11
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	2.10(3)	4(2)					
1Imd	1.87(5)	5(8)					
1Imd	1.95(3)	5(2)	0(2)	0.0292	587.627	86.443	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	6(2)					
1N/O	1.94(7)	11(12)					
1S	2.38(3)	0(3)					
1S	2.58(3)	1(2)					
1Imd	1.95(2)	5(2)					
1Imd	2.11(2)	3(2)	1(2)	0.0235	472.054	69.442	13

Table F14. Additional Fits for Co(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaCl and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.12(3)	5(2)	4(5)	0.3679	1315.864	78.335	3
3N/O	2.12(3)	8(2)	3(3)	0.2650	947.901	56.430	3
4N/O	2.11(2)	10(2)	2(3)	0.2148	768.246	45.735	3
5N/O	2.11(2)	12(2)	1(2)	0.1960	701.006	41.732	3

6N/O	2.10(2)	14(2)	0(2)	0.1958	700.433	41.698	3
7N/O	2.10(2)	16(2)	neg1(2)	0.2064	738.196	43.946	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.23(4)	10(2)	neg14(6)	0.3553	1270.873	75.657	3
3S	2.23(3)	12(2)	neg15(5)	0.2778	993.752	59.159	3
4S	2.23(3)	15(2)	neg16(4)	0.2371	847.906	50.477	3
5S	2.23(3)	17(2)	neg16(4)	0.2159	772.246	45.973	3
6S	2.23(3)	19(2)	neg17(4)	0.2060	736.911	43.869	3
7S	2.23(3)	21(2)	neg17(4)	0.2029	725.801	43.208	3

Co-N(2.0) Co-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.03(2)	2(1)					
1N/O	2.18(2)	3(1)	0(2)	0.1651	590.442	39.900	5
2N/O	2.01(2)	2(1)					
2N/O	2.16(2)	1(1)	neg1(2)	0.1464	523.743	35.393	5
3N/O	2.04(2)	5(2)					
1N/O	2.18(2)	1(1)	neg1(2)	0.1497	535.611	36.195	5
4N/O	2.05(2)	8(2)					
1N/O	2.18(2)	0(2)	neg2(2)	0.1575	563.252	38.063	5
3N/O	2.02(2)	6(2)					
2N/O	2.17(2)	2(2)	neg2(2)	0.1605	574.098	38.796	5
5N/O	2.05(2)	11(2)					
1N/O	2.18(3)	1(2)	neg2(2)	0.1758	628.939	42.502	5
4N/O	2.02(3)	9(3)					
2N/O	2.17(3)	4(2)	neg3(2)	0.1840	658.303	44.486	5
3N/O	2.00(3)	7(3)					
3N/O	2.16(3)	6(3)	neg3(2)	0.1908	682.310	46.109	5
6N/O	2.05(3)	14(3)					
1N/O	2.17(3)	2(3)	neg3(3)	0.1974	706.075	47.715	5
5N/O	2.03(4)	14(5)					
2N/O	2.16(4)	6(4)	neg3(3)	0.2075	742.137	50.152	5
4N/O	2.07(0.19)	22(15)					
3N/O	2.11(7)	12(6)	neg2(4)	0.2117	757.158	51.167	5

Co-S(2.2) Co-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.14(3)	7(2)					
1S	2.28(3)	3(2)	neg20(5)	0.2372	848.408	57.333	5
2S	2.12(3)	8(3)					
2S	2.27(3)	6(2)	neg20(5)	0.2100	751.210	50.765	5
3S	2.26(4)	14(2)					
1S	1.70(9)	23(9)	neg11(6)	0.2323	830.924	56.152	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.14(4)	12(3)					
2S	2.28(4)	8(3)	neg19(5)	0.2039	729.400	49.291	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.24(2)	15(2)					
2S	3.05(4)	12(5)	neg14(3)	0.1766	631.596	42.682	5
3S	2.14(6)	14(5)					
3S	2.28(5)	12(6)	neg19(5)	0.2024	724.003	48.926	5
6S	2.24(2)	19(2)					
1S	3.03(3)	5(3)	neg15(3)	0.1475	527.428	35.642	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.22(4)	16(5)					
3S	2.35(0.18)	27(25)	neg14(6)	0.1995	713.457	48.214	5

Co-N(2.0) Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	5(2)					5
1S	2.29(3)	4(2)	neg9(4)	0.2062	737.537	49.841	
1N/O	1.95(3)	2(2)					5
2S	2.26(3)	8(2)	neg12(4)	0.2052	733.862	49.592	
2N/O	1.98(4)	7(3)					
2S	2.28(3)	10(2)	neg11(4)	0.1921	687.118	46.434	5
3N/O	2.02(3)	9(2)					
1S	2.30(3)	6(2)	neg7(4)	0.1879	671.958	45.409	5

1N/O 3S	2.56(0.11) 2.21(4)	6(9) 12(2)	neg17(6)	0.2530	904.872	61.149	5
1N/O 4S			No Fit	No Fit	No Fit	No Fit	5
4N/O 1S	2.04(4) 2.31(3)	12(3) 8(3)	neg6(4)	0.1827	653.323	44.150	5
2N/O 3S	1.98(5) 2.28(4)	9(4) 14(3)	neg11(5)	0.1936	692.308	46.784	5
3N/O 2S	2.01(5) 2.29(4)	11(3) 12(3)	neg9(5)	0.1901	679.925	45.948	5
5N/O 1S	2.13(2) 2.75(4)	12(2) 11(6)	3(2)	0.1683	602.070	40.686	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.04(7) 2.30(4)	14(4) 14(6)	neg7(5)	0.1900	679.584	45.925	5
2N/O 4S	1.35(0.18) 2.24(4)	32(27) 15(2)	neg14(6)	0.2277	814.501	55.042	5
3N/O 3S	2.01(7) 2.28(5)	13(5) 16(5)	neg10(6)	0.1943	695.102	46.973	5
6N/O 1S			No Fit	No Fit	No Fit	No Fit	5
1N/O 6S	1.37(0.31) 2.23(4)	30(50) 19(2)	neg16(5)	0.2050	733.225	49.549	5
5N/O 2S	2.07(7) 2.29(4)	17(6) 17(9)	neg6(6)	0.1897	678.541	45.854	5
2N/O 5S	2.80(9) 2.25(3)	13(14) 17(2)	neg13(4)	0.1995	713.670	48.228	5
4N/O 3S	2.05(7) 2.29(5)	16(7) 19(8)	neg8(6)	0.1941	694.153	46.909	5
3N/O 4S			No Fit	No Fit	No Fit	No Fit	5

Co-N(2.0) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.10(3)	15(4)					
1Imd	2.10(7)	9(9)	0(2)	0.1530	652.020	44.062	5
4N/O	2.10(2)	16(3)					
1Imd	2.00(1)	0(1)					
1Imd	2.16(1)	1(1)	neg1(1)	0.0612	218.858	17.101	7
3N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
2N/O	2.10(2)	7(3)					
1Imd	1.90(8)	6(15)					
1Imd	2.10(6)	5(8)					
1Imd	2.22(5)	2(8)					
1Imd	1.98(5)	4(7)	neg2(2)	0.0511	185.665	20.763	11
1N/O	2.10(3)	2(4)					
1Imd	1.91(5)	2(11)					
1Imd	2.12(4)	9(8)					
1Imd	2.00(4)	8(9)					
1Imd	1.93(0.43)	44(190)					
1Imd	2.24(4)	6(7)	neg2(3)	0.0552	197.590	29.067	13
4N/O	2.10(3)	12(4)					
1Imd	2.11(7)	10(10)	1(2)	0.1579	564.691	38.160	5
3N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7
2N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.10(3)	2(3)					
1Imd	2.00(4)	7(6)					
1Imd	2.24(3)	5(5)					
1Imd	2.12(3)	8(6)					
1Imd	1.91(5)	1(8)	neg2(2)	0.0561	200.512	22.791	11
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

3N/O	2.12(2)	5(2)					
1Imd	1.97(2)	1(2)	neg2(2)	0.1810	647.412	43.750	5
2N/O	2.10(2)	7(3)					
1Imd	2.16(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0695	248.452	19.414	7
1N/O	2.10(3)	2(3)					
1Imd	1.96(2)	2(2)					
1Imd	2.21(2)	3(4)					
1Imd	2.09(3)	4(4)	neg1(2)	0.0684	244.587	22.651	9
0N/O							
1Imd	2.24(2)	8(4)					
1Imd	2.02(3)	11(4)					
1Imd	1.92(3)	5(4)					
1Imd	2.13(2)	11(4)	neg1(2)	0.1160	415.012	38.435	9
2N/O	2.12(2)	2(2)					
1Imd	1.98(2)	1(2)	neg2(3)	0.2309	825.767	55.803	5
1N/O	2.09(3)	2(3)					
1Imd	2.00(2)	1(1)					
1Imd	2.16(2)	2(1)	0(2)	0.1158	414.252	32.369	7
0N/O							
1Imd	1.97(2)	4(3)					
1Imd	2.08(2)	7(3)					
1Imd	2.20(2)	5(3)	neg1(2)	0.1548	553.624	43.259	7

Co-N(2.0) Co-S(2.2) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
4N/O	2.09(6)	17(6)					
1S	2.30(2)	7(3)					
1Imd	1.99(3)	5(3)	neg5(3)	0.1224	521.452	40.745	7
3N/O	2.10(3)	13(6)					
1S	2.34(0.11)	28(24)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg2(1)	0.0541	193.602	17.930	9
2N/O	2.10(4)	9(4)					
1S	2.35(7)	20(15)					
1Imd	1.99(3)	0(3)					
1Imd	2.15(3)	1(3)					
1Imd	1.95(0.15)	12(20)	neg3(3)	0.0467	166.957	18.977	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(6)	17(6)					
1S	2.30(2)	8(3)					
1Imd	1.99(3)	5(3)	neg5(3)	0.1243	444.684	34.747	7
3N/O	2.10(3)	13(5)					
1S	2.37(0.14)	34(30)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0542	193.790	17.947	9
2N/O	2.10(4)	8(4)					
1S	2.36(7)	21(16)					
1Imd	1.99(4)	0(3)					
1Imd	1.95(0.15)	12(20)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0465	166.433	18.917	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(6)	16(6)					
1S	2.30(3)	8(3)					
1Imd	1.98(3)	5(3)	neg5(3)	0.1261	450.926	35.234	7
3N/O	2.10(3)	14(4)					
1S	2.40(0.16)	38(34)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0539	192.955	17.870	9
2N/O	2.10(3)	8(4)					
1S	2.37(7)	23(17)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	0(3)					
1Imd	1.96(0.15)	12(21)	neg3(2)	0.0463	165.550	18.817	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(5)	16(6)					
1S	2.30(3)	8(3)					
1Imd	1.98(4)	5(3)	neg6(4)	0.1275	455.928	35.625	7
3N/O	2.10(3)	12(4)					
1S	2.42(0.17)	40(36)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0535	191.411	17.727	9
2N/O	2.10(3)	8(4)					
1S	2.38(8)	25(19)	neg3(2)	0.046	164.505	18.698	11

1Imd	1.99(4)	0(3)					
1Imd	2.15(3)	1(3)					
1Imd	1.97(0.16)	12(22)					

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(2)	10(2)					
1S	2.75(4)	12(5)					
1Imd	2.20(3)	3(3)	2(2)	0.1317	470.965	36.800	7
3N/O	2.10(3)	12(4)					
1S	2.44(0.18)	42(36)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0532	190.416	17.635	9
2N/O	2.10(3)	8(4)					
1S	2.39(8)	27(20)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	0(3)					
1Imd	1.97(0.16)	12(22)	neg3(2)	0.0458	163.648	18.601	11

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	8(4)					
2S	2.29(4)	18(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.1236	441.935	34.532	7
2N/O	2.10(3)	8(4)					
2S	2.38(8)	33(12)					
1Imd	1.98(2)	0(1)					
1Imd	2.15(2)	1(1)	neg2(1)	0.0515	184.369	17.075	9
1N/O	2.09(3)	3(3)					
2S	2.38(5)	26(11)					
1Imd	2.16(4)	1(3)					
1Imd	2.00(0.11)	1(5)					
1Imd	1.98(0.19)	7(23)	neg3(2)	0.0435	155.489	17.673	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	7(4)					
2S	2.29(4)	19(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.124	443.355	34.643	7
2N/O	2.10(3)	8(4)					
2S	2.40(8)	36(13)	neg2(1)	0.0517	184.762	17.111	9

1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)					
1N/O	2.09(3)	3(3)					
2S	2.39(5)	28(11)					
1Imd	2.17(4)	1(3)					
1Imd	2.01(0.18)	1(6)					
1Imd	1.98(0.24)	5(27)	neg3(2)	0.0434	155.224	17.643	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	7(3)					
2S	2.30(4)	19(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.1245	445.292	34.794	7
2N/O	2.10(3)	8(3)					
2S	2.42(8)	37(14)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg2(1)	0.0514	183.787	17.021	9
1N/O	2.09(3)	3(3)					
2S	2.40(5)	30(11)					
1Imd	2.02(0.31)	1(10)					
1Imd	2.17(4)	1(3)					
1Imd	1.97(0.34)	4(34)	neg3(2)	0.0431	154.186	17.525	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	7(3)					
2S	2.30(4)	20(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.1248	446.571	34.894	7
2N/O	2.09(3)	8(3)					
2S	2.43(8)	39(14)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg2(1)	0.0509	182.057	16.860	9
1N/O	2.09(3)	3(3)					
2S	2.41(6)	31(12)					
1Imd	2.03(0.27)	1(19)					
1Imd	1.97(0.28)	3(27)					
1Imd	2.17(3)	1(4)	neg3(2)	0.0427	152.804	17.368	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	6(2)					
2S	2.71(8)	29(13)					
1Imd	2.20(2)	1(2)	3(2)	0.1557	556.990	43.522	7

2N/O	2.09(3)	8(3)					
2S	2.44(9)	40(15)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg2(1)	0.0506	181.153	16.777	9
1N/O	2.09(3)	3(3)					
2S	2.41(6)	32(12)					
1Imd	2.17(3)	1(4)					
1Imd	2.04(0.17)	1(18)					
1Imd	1.96(0.18)	2(19)	neg3(2)	0.0424	151.705	17.243	11

Co-N(2.0) Co-S(2.2) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	19(10)					
1S	2.44(6)	9(7)					
1S	2.27(3)	4(3)					
1Imd	1.98(3)	3(2)	neg6(3)	0.105	375.635	34.788	9
2N/O	2.07(3)	9(4)					
1S	2.66(6)	13(6)					
1S	2.41(5)	11(5)					
1Imd	2.15(2)	1(1)					
1Imd	2.00(2)	0(1)	neg1(1)	0.0421	150.622	17.120	11
1N/O	2.07(3)	3(4)					
1S	2.35(4)	9(6)					
1S	2.58(0.10)	19(14)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	0(3)					
1Imd	1.96(0.16)	12(22)	neg3(2)	0.0372	133.034	19.570	11

Co-N(2.0) Co-S(2.2) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(7)	18(9)					
1S	2.44(6)	9(6)					
1S	2.28(3)	4(3)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1063	380.182	35.209	9
2N/O	2.07(3)	8(4)					
1S	2.66(6)	12(6)					
1S	2.42(5)	11(5)					
1Imd	2.00(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0412	147.497	16.765	11
1N/O	2.07(3)	3(4)					
1S	2.35(4)	9(6)					
1S	2.59(9)	19(13)	neg3(2)	0.0362	129.416	19.038	11

1Imd	1.96(0.16)	13(23)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)					

Co-N(2.0) Co-S(2.2) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	21(10)					
1S	2.27(3)	4(2)					
1S	2.44(7)	12(8)					
1Imd	1.98(2)	3(2)	neg6(3)	0.1021	365.072	33.810	9
2N/O	2.07(3)	10(5)					
1S	2.37(5)	11(5)					
1S	2.65(7)	16(8)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.04	142.918	16.245	11
1N/O	2.07(3)	3(4)					
1S	2.35(4)	10(6)					
1S	2.59(9)	20(13)					
1Imd	1.97(0.16)	13(23)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0353	126.382	18.591	11

Co-N(2.0) Co-S(2.2) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	20(10)					
1S	2.27(3)	4(2)					
1S	2.44(7)	13(8)					
1Imd	1.98(2)	3(2)	neg6(3)	0.1014	362.644	33.585	9
2N/O	2.07(4)	11(5)					
1S	2.37(5)	12(5)					
1S	2.64(7)	17(8)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0393	140.544	15.975	11
1N/O	2.07(4)	3(4)					
1S	2.35(4)	10(6)					
1S	2.59(9)	20(13)					
1Imd	1.97(0.17)	14(23)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0347	124.012	18.243	11

Co-N(2.0) Co-S(2.3) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

3N/O	2.07(7)	18(9)					
1S	2.44(7)	10(7)					
1S	2.28(3)	4(3)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1058	378.376	35.042	9
2N/O	2.07(3)	9(4)					
1S	2.39(5)	12(5)					
1S	2.66(6)	14(7)					
1Imd	2.15(2)	1(1)					
1Imd	2.00(2)	0(1)	neg1(1)	0.0397	142.076	16.149	11
1N/O	2.07(3)	3(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	18(11)					
1Imd	1.99(4)	1(2)					
1Imd	1.96(0.15)	12(21)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0353	126.205	18.565	11

Co-N(2.0) Co-S(2.3) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	19(10)					
1S	2.27(3)	5(2)					
1S	2.44(7)	12(8)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1031	368.639	34.140	9
2N/O	2.07(3)	10(4)					
1S	2.39(5)	12(5)					
1S	2.66(6)	14(7)					
1Imd	2.00(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0389	139.157	15.817	11
1N/O	2.07(3)	3(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	18(11)					
1Imd	1.96(0.15)	12(21)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0344	123.084	18.106	11

Co-N(2.0) Co-S(2.3) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	19(10)					
1S	2.27(3)	5(2)					
1S	2.45(7)	13(8)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1023	366.048	33.900	9
2N/O	2.07(3)	10(5)					
1S	2.38(5)	12(5)					
1S	2.65(6)	15(7)	neg1(1)	0.0383	136.859	15.556	11

1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)					
1N/O	2.07(3)	3(3)					
1S	2.36(4)	10(6)					
1S	2.60(8)	19(11)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)					
1Imd	1.96(0.15)	13(21)	neg3(2)	0.0337	120.655	17.749	11

Co-N(2.0) Co-S(2.4) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(7)	18(9)					
1S	2.28(3)	5(2)					
1S	2.45(7)	12(8)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1042	372.641	34.511	9
2N/O	2.07(3)	9(4)					
1S	2.40(5)	12(5)					
1S	2.66(6)	13(6)					
1Imd	2.00(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.038	135.944	15.452	11
1N/O	2.07(3)	3(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	17(10)					
1Imd	1.96(0.14)	12(20)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	1(2)	neg3(2)	0.0337	120.642	17.747	11

Co-N(2.0) Co-S(2.4) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	3N/O	2.07(7)	18(9)				
1S	1S	2.28(3)	5(2)				
1S	1S	2.45(7)	13(8)				
1Imd	1Imd	1.98(3)	3(2)	neg6(3)	0.1034	369.900	9
2N/O	2N/O	2.07(3)	10(4)				
1S	1S	2.39(5)	12(5)				
1S	1S	2.66(6)	14(6)				
1Imd	1Imd	2.00(2)	0(1)				
1Imd	1Imd	2.15(2)	1(1)	neg1(1)	0.0374	133.740	11
1N/O	1N/O	2.07(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	18(10)					
1Imd	2.15(3)	1(3)					
1Imd	1.96(0.14)	12(20)	3(3)	neg3(2)	0.033	118.171	11

1Imd	1.99(4)	1(2)					

Co-N(2.0) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(7)	18(9)					
1S	2.46(7)	12(7)					
1S	2.28(3)	5(3)					
1Imd	1.98(3)	3(2)	neg7(3)	0.1054	377.150	34.928	9
2N/O	2.07(3)	9(4)					
1S	2.40(5)	12(5)					
1S	2.67(5)	13(6)					
1Imd 0°	2.15(2)	1(1)					
1Imd 0°	2.00(2)	0(1)	neg1(1)	0.0365	130.623	14.847	11
2N/O	2.07(4)	11(5)					
1S	2.40(5)	12(5)					
1S	2.68(6)	14(6)					
1Imd 0°	2.15(2)	2(1)					
1Imd 5°	2.00(2)	1(1)	neg1(1)	0.0374	133.832	15.212	11
2N/O	2.02(7)	16(11)					
1S	2.51(8)	12(8)					
1S	2.32(4)	6(4)					
1Imd 0°	1.97(2)	3(2)					
1Imd 10°	2.09(4)	2(3)	neg5(2)	0.0613	219.089	24.903	11
2N/O	2.03(8)	17(12)					
1S	2.50(8)	14(10)					
1S	2.31(4)	7(5)					
1Imd 5°	1.97(2)	2(2)					
1Imd 10°	2.10(4)	2(2)	neg5(2)	0.0595	212.666	24.172	11
1N/O	2.07(3)	3(3)					
1S	2.37(4)	10(5)					
1S	2.61(7)	17(9)					
1Imd	1.96(0.14)	12(20)					
1Imd	1.99(4)	1(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0326	116.576	17.149	13

Co-N(2.2) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(8)	19(10)					
1S	2.45(8)	13(9)					
1S	2.28(3)	5(3)					
1Imd	1.98(3)	3(2)	neg7(3)	0.1041	372.421	34.490	9
2N/O	2.08(3)	10(4)	neg2(1)	0.0356	127.368	14.477	11

1S	2.41(5)	13(5)					
1S	2.68(5)	12(5)					
1Imd 0°	2.15(2)	1(1)					
1Imd 0°	1.99(2)	0(1)					
2N/O	2.08(4)	12(5)					
1S	2.41(6)	14(6)					
1S	2.69(6)	13(6)					
1Imd 0°	2.15(2)	1(1)					
1Imd 5°	2.00(2)	1(1)	neg1(1)	0.0371	132.615	15.074	11
2N/O	2.04(9)	19(14)					
1S	2.51(9)	13(9)					
1S	2.31(4)	6(5)					
1Imd 0°	1.97(2)	3(2)					
1Imd 10°	2.09(4)	2(3)	neg6(2)	0.0621	221.978	25.231	11
2N/O	2.05(9)	20(14)					
1S	2.50(9)	15(11)					
1S	2.31(4)	7(5)					
1Imd 5°	1.97(2)	2(2)					
1Imd 10°	2.10(4)	2(2)	neg5(3)	0.0602	215.435	24.487	11
1N/O	2.08(3)	3(3)					
1S	2.38(4)	10(6)					
1S	2.63(7)	16(8)					
1Imd	1.99(3)	1(2)					
1Imd	1.98(0.18)	15(24)					
1Imd	2.15(3)	1(2)	neg3(2)	0.0323	115.496	16.990	13

Co-N(2.0) Co-N(2.2) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(5)	5(6)					
1N/O	2.11(3)	0(3)					
1S	2.66(5)	8(4)					
1S	2.42(4)	8(4)					
1Imd 0°	2.00(2)	2(2)					
1Imd 0°	2.15(2)	2(1)	neg2(2)	0.0259	92.765	13.646	13
1N/O	1.95(4)	3(5)					
1N/O	2.12(2)	1(3)					
1S	2.43(4)	9(4)					
1S	2.68(5)	10(4)					
1Imd 0°	2.16(2)	1(1)					
1Imd 5°	2.01(2)	2(2)	neg2(2)	0.0264	94.424	13.890	13
1N/O	1.97(2)	1(1)					
1N/O	2.15(3)	0(3)					
1S	2.74(6)	10(6)	0(2)	0.0349	124.764	18.353	13

1S	2.47(7)	15(7)					
1Imd 0°	2.15(6)	9(8)					
1Imd 10°	2.10(3)	2(3)					
1N/O	1.97(2)	1(1)					
1N/O	2.15(3)	0(3)					
1S	2.74(6)	11(6)					
1S	2.46(7)	15(7)					
1Imd 5°	2.15(6)	8(8)					
1Imd 10°	2.10(3)	2(3)	0(2)	0.0362	129.633	19.070	13

Table G.13. Additional Fits for Ni(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaCl and 10 % Glycerol at pH 7.0.

Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	10(1)	5(4)	0.2732	5494.488	327.095	3
3N/O	2.07(1)	3(1)	5(2)	0.1788	3596.559	214.108	3
4N/O	2.08(1)	5(1)	4(2)	0.1401	2817.942	167.756	3
5N/O	2.08(1)	7(1)	4(2)	0.1354	2722.610	162.081	3
6N/O	2.08(1)	9(1)	3(2)	0.1510	3035.995	180.737	3
7N/O	2.08(2)	11(1)	3(2)	0.1778	3575.075	212.829	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(2)	5(1)	neg17(6)	0.2975	5983.760	356.222	3
3S	2.17(2)	8(1)	neg17(5)	0.2513	5053.699	300.854	3
4S	2.17(2)	11(1)	neg17(4)	0.2377	4780.260	284.576	3
5S	2.18(3)	13(1)	neg17(4)	0.2385	4796.296	285.530	3
6S	2.18(3)	15(2)	neg17(4)	0.2456	4940.403	294.109	3
7S	2.18(3)	17(2)	neg17(4)	0.2554	5137.486	305.842	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.03(2)	1(2)					
1N/O	2.16(2)	3(2)	4(2)	0.1482	2979.785	201.366	5
2N/O	2.03(3)	2(3)					
2N/O	2.14(3)	2(4)	4(2)	0.1316	2646.506	178.844	5
3N/O	2.05(2)	2(2)					
1N/O	2.17(4)	0(4)	4(2)	0.1320	2654.462	179.382	5

4N/O	2.08(2)	5(1)					
1N/O	2.30(9)	11(15)	6(2)	0.1217	2446.847	165.351	5
3N/O	2.07(1)	3(1)					
2N/O	2.21(9)	17(14)	6(2)	0.1237	2486.830	168.053	5
5N/O	2.09(1)	7(1)					
1N/O	2.37(5)	6(6)	6(2)	0.1143	2298.130	155.302	5
4N/O	2.08(1)	5(1)					
2N/O	2.32(6)	14(10)	7(2)	0.1117	2246.329	151.801	5
3N/O	2.08(1)	3(1)					
3N/O	2.25(7)	22(120	7(2)	0.1167	2347.532	158.640	5
6N/O	2.09(1)	9(1)					
1N/O	2.39(4)	3(4)	6(2)	0.1196	2404.888	162.516	5
5N/O	2.09(1)	6(1)					
2N/O	2.37(4)	10(6)	7(1)	0.1079	2170.971	146.708	5
4N/O	2.09(1)	5(1)					
3N/O	2.33(5)	18(8)	8(2)	0.1086	2185.088	147.663	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.15(3)	5(3)					
1S	2.29(7)	5(7)	neg14(6)	0.2398	4822.496	325.892	5
2S	2.17(2)	5(2)					
2S	2.31(6)	12(8)	neg11(5)	0.2114	4251.883	287.331	5
3S	2.18(3)	7(2)					
1S	2.37(6)	7(7)	neg12(5)	0.2134	4292.269	290.060	5
4S	2.20(3)	9(1)					
1S	2.42(4)	6(5)	neg11(4)	0.1934	3889.767	262.860	5
3S	2.19(2)	7(1)					
2S	2.38(5)	11(6)	neg10(4)	0.1860	3741.517	252.842	5
5S	2.17(3)	12(2)					
1S	1.43(0.18)	33(40)	neg18(5)	0.2333	4692.873	317.132	5
4S	2.21(2)	9(1)					
2S	2.42(4)	10(4)	neg9(3)	0.1665	3348.563	226.287	5
3S	2.38(4)	14(5)					
3S	2.19(2)	7(2)	neg9(4)	0.1781	3582.848	242.119	5

6S	2.14(3)	12(2)					
1S	1.90(4)	9(5)	neg22(5)	0.2206	4435.632	299.748	5
5S	2.22(2)	11(1)					
2S	2.45(3)	8(3)	neg9(3)	0.1535	3086.167	208.555	5
4S	2.21(2)	9(1)					
3S	2.43(3)	12(3)	neg8(3)	0.1450	2915.267	197.006	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(3)	2(2)					5
1S	2.27(5)	6(4)	neg2(5)	0.2322	4669.902	315.580	
1N/O	1.99(4)	1(3)					5
2S	2.22(4)	7(3)	neg9(6)	0.2541	5109.847	345.310	
2N/O	2.07(2)	1(1)					
2S	2.50(9)	24(13)	5(3)	0.1995	4012.759	271.172	5
3N/O	2.08(1)	3(1)					
1S	2.58(4)	10(5)	6(2)	0.1297	2608.297	176.262	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O	1.75(5)	7(7)					
4S	2.16(2)	10(1)	neg20(4)	0.2192	4409.197	297.962	5
4N/O	2.08(1)	5(1)					
1S	2.59(3)	9(4)	6(1)	0.0862	1732.886	117.104	5
2N/O	4.14(0.12)	3(12)					
3S	2.17(2)	8(1)	neg16(5)	0.2410	4847.641	327.591	5
3N/O	2.08(1)	3(1)					
2S	2.57(4)	19(6)	6(2)	0.1139	2290.289	154.772	5
5N/O	2.08(2)	7(1)					
1S	1.94(0.10)	29(29)	5(2)	0.1291	2595.962	175.428	5
1N/O	2.29(5)	1(4)					
5S	2.20(3)	12(2)	neg15(5)	0.2246	4517.055	305.251	5
4N/O	2.08(1)	5(1)					
2S	2.59(3)	16(4)	6(1)	0.0761	1530.630	103.436	5
2N/O	2.68(4)	5(4)	neg13(3)	0.1761	3540.753	239.275	5

4S	2.19(2)	11(1)					
3N/O	1.82(0.10)	20(17)					
3S	2.17(3)	8(2)	neg19(6)	0.2266	4557.384	307.976	5
6N/O	2.07(3)	7(2)					
1S	2.00(0.11)	15(13)	4(2)	0.1307	2628.715	177.642	5
1N/O	3.17(0.10)	3(10)					
6S	2.18(3)	15(2)	neg17(4)	0.2211	4445.891	300.442	5
5N/O	2.08(1)	7(1)					
2S	1.95(6)	34(18)	6(2)	0.1237	2488.387	168.159	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.83(0.11)	24(18)					
3S	2.17(3)	8(2)	neg19(7)	0.2248	4522.085	305.591	5
3N/O	3.18(6)	6(6)					
4S	2.17(2)	10(1)	neg17(4)	0.1787	3593.976	242.871	5

Ni-N(2.0) Ni-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.08(2)	7(2)					
1Imd	1.97(8)	11(11)	2(2)	0.1218	2356.722	159.261	5
4N/O	2.08(2)	6(2)					
1Imd	1.90(6)	8(12)					
1Imd	2.04(6)	5(9)	1(2)	0.1043	2098.271	163.955	7
3N/O	2.07(2)	3(2)					
1Imd	1.98(3)	3(4)					
1Imd	1.85(4)	2(5)					
1Imd	2.12(4)	1(4)	0(2)	0.0965	1940.163	179.680	9
2N/O	2.07(2)	1(2)					
1Imd	2.21(0.29)	8(48)					
1Imd	2.12(0.11)	3(12)					
1Imd	1.87(0.10)	1(10)					
1Imd	1.99(9)	4(10)	2(4)	0.1063	2138.796	243.104	11
1N/O	2.08(3)	3(3)					
1Imd	2.37(8)	8(9)					
1Imd	2.24(6)	16(5)					
1Imd	2.01(5)	16(5)					
1Imd	2.12(6)	18(5)					
1Imd	1.90(5)	9(5)	5(3)	0.1128	2267.669	333.586	13

4N/O	2.08(2)	6(2)					
1Imd	2.02(6)	7(7)	3(2)	0.1114	2240.241	151.390	5
3N/O	2.08(2)	4(2)					
1Imd	2.10(0.12)	8(18)					
1Imd	1.97(9)	6(10)	3(3)	0.1079	2170.711	169.615	7
2N/O	2.07(2)	1(2)					
1Imd	2.15(4)	2(4)					
1Imd	2.01(4)	3(4)					
1Imd	1.89(6)	2(7)	2(2)	0.1103	2218.211	205.431	9
1N/O	2.07(3)	2(3)					
1Imd	2.20(4)	9(4)					
1Imd	1.96(4)	11(4)					
1Imd	1.85(4)	5(5)					
1Imd	2.08(4)	12(4)	1(3)	0.1335	2684.105	305.086	11
0N/O							
1Imd	1.88(6)	9(8)					
1Imd	1.98(6)	15(8)					
1Imd	2.20(8)	13(12)					
1Imd	2.28(0.20)	1(40)					
1Imd	2.09(6)	16(9)	4(3)	0.2463	4953.895	563.080	11
3N/O	2.09(2)	4(2)					
1Imd	2.03(6)	5(6)	4(2)	0.1225	2464.494	166.544	5
2N/O	2.08(2)	1(2)					
1Imd	2.15(4)	1(4)					
1Imd	1.99(3)	1(3)	4(2)	0.1240	2494.573	194.921	7
1N/O	2.07(2)	2(2)					
1Imd	2.17(4)	4(4)					
1Imd	2.04(6)	3(7)					
1Imd	1.94(7)	0(11)	3(3)	0.1489	2995.272	277.395	9
0N/O							
1Imd	2.21(4)	10(5)					
1Imd	1.99(3)	13(4)					
1Imd	1.88(4)	7(5)					
1Imd	2.10(3)	14(4)	3(2)	0.2579	5186.616	480.338	9
2N/O	2.08(3)	2(2)					
1Imd	2.04(6)	4(5)	4(3)	0.1713	3445.923	232.866	5
1N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

0N/O							
1Imd	2.06(7)	5(13)					
1Imd	2.17(6)	4(9)					
1Imd	1.97(9)	2(15)	4(3)	0.2950	5932.920	463.587	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.58(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0553	1112.935	86.963	7
3N/O	2.09(1)	4(2)					
1S	2.59(3)	8(3)					
1Imd	2.18(4)	3(4)					
1Imd	2.01(3)	2(3)	6(1)	0.0514	1033.334	95.698	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	2.21(6)	0(10)					
1Imd	2.08(8)	1(16)					
1Imd	1.97(8)	1(10)	5(2)	0.0617	1240.148	140.960	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.59(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0531	1068.314	83.476	7
3N/O	2.09(1)	4(2)					
1S	2.59(2)	8(3)					
1Imd	2.18(4)	4(4)					
1Imd	2.01(3)	3(3)	5(1)	0.0493	991.415	91.816	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	2.20(6)	0(9)					
1Imd	1.97(0.10)	2(13)					
1Imd	2.07(9)	0(18)	5(2)	0.0588	1183.547	134.527	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.59(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0515	1035.399	80.904	7
3N/O	2.09(1)	4(2)	5(1)	0.0479	963.906	89.268	9

1S	2.59(2)	8(3)					
1Imd	2.01(3)	3(3)					
1Imd	2.17(4)	4(4)					
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	1.96(0.11)	2(15)					
1Imd	2.20(5)	0(8)					
1Imd	2.07(9)	0(17)	5(2)	0.057	1145.370	130.188	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.60(2)	8(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0502	1010.598	78.966	7
3N/O	2.08(1)	4(2)					
1S	2.59(2)	8(3)					
1Imd	2.17(4)	4(4)					
1Imd	2.01(3)	3(3)	5(1)	0.0469	944.130	87.437	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	8(4)					
1Imd	2.06(9)	0(15)					
1Imd	2.19(5)	1(7)					
1Imd	1.96(0.11)	3(15)	4(2)	0.0555	1115.911	126.839	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	7(2)					
1S	2.60(2)	9(3)					
1Imd	2.06(4)	5(4)	5(1)	0.0493	991.533	77.477	7
3N/O	2.08(1)	4(2)					
1S	2.60(2)	8(3)					
1Imd	2.01(3)	3(3)					
1Imd	2.17(4)	4(4)	5(1)	0.0461	926.610	85.814	9
2N/O	2.08(2)	1(2)					
1S	2.58(4)	9(4)					
1Imd	2.05(8)	0(13)					
1Imd	1.96(0.10)	3(15)					
1Imd	2.19(4)	1(6)	4(2)	0.0542	1089.150	123.797	11

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

3N/O	2.09(1)	5(2)					
2S	2.58(3)	16(4)					
1Imd	2.08(4)	6(5)	6(1)	0.0604	1214.643	94.910	7
2N/O	2.08(1)	1(1)					
2S	2.58(3)	15(4)					
1Imd	2.17(2)	1(2)					
1Imd	2.01(2)	0(2)	6(1)	0.0549	1103.446	102.191	9
1N/O	2.07(2)	2(2)					
2S	2.54(6)	17(6)					
1Imd	2.05(5)	5(6)					
1Imd	1.94(5)	1(7)					
1Imd	2.18(4)	5(4)	4(2)	0.083	1669.293	189.739	11

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.59(3)	16(4)					
1Imd	2.08(4)	6(5)	6(1)	0.058	1167.253	91.207	7
2N/O	2.08(1)	1(1)					
2S	2.58(3)	15(4)					
1Imd	2.01(2)	0(2)					
1Imd	2.17(2)	0(2)	6(10	0.0529	1064.611	98.595	9
1N/O	2.07(2)	2(2)					
2S	2.54(5)	17(6)					
1Imd	2.17(3)	5(4)					
1Imd	1.94(5)	1(7)					
1Imd	2.05(4)	5(5)	4(2)	0.0795	1599.147	181.766	11

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.59(3)	16(4)					
1Imd	2.07(4)	6(5)	6(1)	0.0567	1140.063	89.082	7
2N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.59(3)	17(4)					
1Imd	2.07(4)	6(5)	5(1)	0.056	1126.948	88.058	7
2N/O	2.08(1)	1(1)					
2S	2.59(3)	16(4)					
1Imd	2.16(2)	0(2)					
1Imd	2.00(2)	0(2)	5(1)	0.0523	1051.269	97.359	9
1N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	5(2)					
2S	2.60(3)	17(4)					
1Imd	2.07(4)	6(5)	5(1)	0.0556	1117.943	87.354	7
2N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.06(2)	2(2)					
2S	2.54(5)	19(6)					
1Imd	2.04(4)	5(4)					
1Imd	2.17(3)	5(3)					
1Imd	1.93(4)	1(6)	3(2)	0.0743	1495.056	169.934	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.62(3)	5(3)					
1S	2.45(5)	11(6)					
1Imd	2.05(5)	6(5)	5(1)	0.0469	87.309	942.749	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	6(4)					
1S	2.60(3)	3(2)					
1Imd	2.13(3)	0(2)	4(2)	0.0341	77.960	685.881	11

1Imd	1.97(3)	0(2)					
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.89(7)	6(12)					
1Imd	1.95(4)	4(3)	1(2)	0.0331	98.013	666.275	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.43(6)	12(7)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.045	905.017	83.815	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	6(4)					
1S	2.60(3)	3(2)					
1Imd	2.13(3)	1(2)					
1Imd	1.97(3)	0(2)	4(2)	0.0341	686.000	77.974	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	1.95(4)	4(3)					
1Imd	1.89(6)	5(10)					
1Imd	2.11(3)	4(2)	0(2)	0.0313	628.650	92.478	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.42(6)	13(7)					
1S	2.619(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0445	894.140	82.807	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.13(3)	1(2)	3(2)	0.0339	681.773	77.493	11
1N/O	2.04(2)	6(2)					
1S	2.34(3)	0(3)					
1S	2.55(3)	1(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.88(6)	5(10)					
1Imd	1.95(4)	4(2)	0(2)	0.0294	592.244	87.122	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.42(6)	13(8)					
1S	2.61(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.044	884.804	81.943	9
2N/O	2.07(1)	0(1)					
1S	2.39(4)	7(5)					
1S	2.60(3)	4(2)					
1Imd	2.12(3)	1(3)					
1Imd	1.96(3)	0(2)	3(2)	0.0336	675.221	76.748	11
1N/O	2.04(2)	6(2)					
1S	2.34(3)	0(3)					
1S	2.55(3)	1(2)					
1Imd	1.88(6)	5(9)					
1Imd	1.95(4)	4(2)					
1Imd	2.11(3)	4(2)	0(2)	0.0279	561.056	82.534	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.62(3)	5(3)					
1S	2.45(5)	12(7)					
1Imd	2.05(5)	6(5)	5(1)	0.0454	913.046	84.558	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	6(4)					
1S	2.60(3)	3(2)					
1Imd	2.13(3)	0(2)					
1Imd	1.96(3)	0(2)	3(2)	0.0335	673.515	76.554	11
1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	1.89(6)	5(11)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(4)	4(2)	0(2)	0.0308	620.411	91.266	11

Ni-N(2.2) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	0(1)					
1S	2.61(3)	2(2)					
1S	2.43(4)	6(4)	3(1)	0.0317	637.618	72.474	11

1Imd	1.97(2)	0(2)					
1Imd	2.13(3)	0(2)					
1N/O	2.05(2)	6(2)					
1S	2.56(3)	1(3)					
1S	2.37(3)	0(4)					
1Imd	1.95(4)	5(3)					
1Imd	2.11(3)	4(2)					
1Imd	1.89(7)	5(10)	0(2)	0.0343	688.909	101.342	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.43(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0443	890.838	82.501	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.0333	669.891	76.143	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.89(6)	5(10)					
1Imd	1.95(4)	4(2)	0(2)	0.029	583.969	85.905	11

Ni-N(2.2) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.42(4)	7(5)					
1S	2.61(3)	3(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.13(3)	1(3)	3(1)	0.0327	658.585	74.857	11
1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	1.87(6)	5(8)					
1Imd	1.95(3)	5(2)					
1Imd	2.10(3)	4(2)	0(2)	0.031	624.037	91.799	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.42(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0439	882.159	81.698	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.033	664.144	75.489	11
1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.88(6)	5(10)					
1Imd	1.95(3)	4(2)	0(2)	0.0275	552.635	81.295	11

Ni-N(2.2) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(1)	1(1)					
1S	2.41(4)	8(5)					
1S	2.61(3)	4(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.12(3)	1(3)	3(1)	0.0325	654.174	74.356	11
1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.56(3)	1(2)					
1Imd	2.10(3)	4(2)					
1Imd	1.87(5)	5(8)					
1Imd	1.95(3)	5(2)	0(2)	0.0293	589.901	86.778	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.42(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0439	882.159	81.698	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.033	664.144	75.489	11

1N/O	2.04(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.55(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.88(6)	5(10)					
1Imd	1.95(3)	4(2)	0(2)	0.0275	552.635	81.295	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.44(6)	13(8)					
1S	2.62(3)	6(3)					
1Imd	2.05(5)	6(5)	4(1)	0.0442	889.665	82.393	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	7(4)					
1S	2.60(3)	3(2)					
1Imd	2.12(3)	1(2)					
1Imd	1.96(3)	0(2)	3(2)	0.033	663.253	75.388	11
2N/O	2.08(1)	1(2)					
1S	2.42(4)	8(5)					
1S	2.61(3)	4(3)					
1Imd 0°	2.12(3)	1(3)					
1Imd 5°	1.97(3)	0(2)	4(1)	0.0338	680.355	77.332	11
2N/O	2.06(3)	3(3)					
1S	2.39(5)	10(7)					
1S	2.59(3)	5(3)					
1Imd 0°	2.02(8)	9(8)					
1Imd 10°	2.08(5)	3(6)	3(2)	0.0384	771.888	87.736	11
2N/O	2.06(3)	3(3)					
1S	2.39(5)	10(7)					
1S	2.59(3)	5(3)					
1Imd 5°	2.02(9)	8(8)					
1Imd 10°	2.09(5)	3(5)	3(2)	0.0394	791.951	90.016	11
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	1.89(6)	5(10)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(4)	4(2)	0(2)	0.029	583.773	85.876	13

Ni-N(2.2) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)	3(1)	0.0322	646.809	73.519	11

1S	2.42(4)	7(5)					
1S	2.61(3)	3(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.12(3)	1(3)					
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	1.95(3)	5(2)					
1Imd	1.88(6)	5(8)					
1Imd	2.11(3)	4(2)	0(2)	0.0309	622.370	91.554	11

Ni-N(2.2) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(3)	6(3)					
1N/O	2.16(5)	5(5)					
1S	2.39(0.14)	18(27)					
1S	2.57(6)	6(7)					
1Imd	1.93(4)	1(4)					
1Imd	2.10(4)	2(4)	3(2)	0.0303	609.696	89.690	13

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.43(6)	14(8)					
1S	2.62(3)	6(3)					
1Imd	2.04(5)	6(5)	4(1)	0.0438	881.627	81.648	9
2N/O	2.07(1)	0(1)					
1S	2.40(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	1.96(3)	0(2)					
1Imd	2.12(3)	1(2)	3(2)	0.0327	658.034	74.795	11
2N/O	2.08(1)	1(2)					
1S	2.42(5)	9(5)					
1S	2.61(3)	4(3)					
1Imd 0°	2.12(3)	1(3)					
1Imd 5°	1.97(3)	0(2)	4(2)	0.0338	680.523	77.351	11
2N/O	2.06(3)	3(3)					
1S	2.38(5)	9(6)					
1S	2.59(3)	5(3)					
1Imd 0°	2.01(8)	9(7)					
1Imd 10°	2.08(5)	3(6)	3(2)	0.0377	757.520	86.103	11
2N/O	2.06(3)	3(3)					
1S	2.39(5)	10(7)					
1S	2.59(3)	5(3)	3(2)	0.0389	781.398	88.817	11

1Imd 5°	2.01(9)	8(8)					
1Imd 10°	2.09(5)	3(5)					
1N/O	2.05(2)	6(2)					
1S	2.35(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(3)	4(2)					
1Imd	1.88(6)	5(10)	0(2)	0.0274	551.623	81.147	13

Ni-N(2.2) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(1)	1(1)					
1S	2.42(4)	8(5)					
1S	2.61(3)	4(2)					
1Imd	1.97(3)	0(2)					
1Imd	2.12(3)	1(3)	3(1)	0.032	643.399	73.131	11
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	1.87(5)	5(8)					
1Imd	2.10(3)	4(2)					
1Imd	1.95(3)	5(2)	0(2)	0.0292	587.576	86.435	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	6(2)					
1N/O	1.94(7)	11(12)					
1S	2.38(3)	0(3)					
1S	2.58(3)	1(2)					
1Imd	1.95(2)	5(2)					
1Imd	2.11(2)	3(2)	1(2)	0.0235	472.054	69.442	13
1N/O	2.11(3)	5(3)					
1N/O	1.99(3)	4(3)					
1S	2.40(5)	5(6)					
1S	2.60(4)	3(4)					
1Imd 0°	1.97(7)	7(7)					
1Imd 10°	2.10(6)	3(6)	2(2)	0.0326	654.856	96.333	13

Ni-N(2.0) Ni-Cl(2.4) Ni-Cl(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	4(2)					
1Cl	2.39(5)	13(7)					
1Cl	2.59(3)	6(3)					
1Imd	2.04(5)	6(5)	4(2)	0.0451	906.107	83.915	9

2N/O	2.06(1)	0(1)					
1Cl	2.37(4)	6(4)					
1Cl	2.57(3)	4(2)					
1Imd	2.11(3)	1(3)					
1Imd	1.95(3)	0(2)	2(2)	0.033	663.374	75.402	11
1N/O	2.04(2)	6(2)					
1Cl	2.32(3)	0(3)					
1Cl	2.53(3)	1(2)					
1Imd	1.88(5)	5(10)					
1Imd	1.95(4)	4(2)					
1Imd	2.10(3)	4(2)	0(2)	0.0255	513.237	75.500	11

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.08(1)	4(2)					
1S	2.62(3)	5(3)					
1S	2.45(6)	13(8)					
1Imd	2.05(5)	6(5)	4(1)	0.0444	893.875	82.783	9
2N/O	2.07(1)	0(1)					
1S	2.41(4)	7(5)					
1S	2.60(3)	3(2)					
1Imd	2.12(3)	1(2)					
1Imd	1.96(3)	0(2)	3(2)	0.0327	656.759	74.650	11
2N/O	2.09(2)	3(2)					
1S	1.82(8)	35(13)					
1S	2.61(2)	9(3)					
1Imd 0°	2.17(3)	2(3)					
1Imd 5°	2.02(3)	1(3)	6(1)	0.0336	675.360	76.764	11
2N/O	2.06(3)	3(3)					
1S	2.59(3)	4(3)					
1S	2.39(5)	10(7)					
1Imd 0°	2.01(8)	8(7)					
1Imd 10°	2.08(5)	3(6)	3(2)	0.0391	785.484	89.281	11
2N/O	2.06(3)	3(3)					
1S	2.60(3)	4(3)					
1S	2.40(5)	10(7)					
1Imd 5°	2.02(8)	8(7)					
1Imd 10°	2.09(5)	3(5)	3(2)	0.04	803.726	91.355	11
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	2.11(3)	4(2)					
1Imd	1.95(3)	4(2)	0(2)	0.0276	554.494	81.569	13

1Imd	1.88(6)	5(9)					

Ni-N(2.2) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.42(4)	7(5)					
1S	2.61(3)	3(2)					
1Imd	2.12(3)	1(3)					
1Imd	1.97(3)	0(2)	3(1)	0.0317	636.960	72.399	11
1N/O	2.05(2)	6(2)					
1S	2.36(3)	0(3)					
1S	2.56(3)	0(2)					
1Imd	2.10(3)	4(2)					
1Imd	1.87(5)	5(8)					
1Imd	1.95(3)	5(2)	0(2)	0.0292	587.627	86.443	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	6(2)					
1N/O	1.94(7)	11(12)					
1S	2.38(3)	0(3)					
1S	2.58(3)	1(2)					
1Imd	1.95(2)	5(2)					
1Imd	2.11(2)	3(2)	1(2)	0.0235	472.054	69.442	13

Table G.14. Additional Fits for Co(II) E63A-RcnR in Buffer with 20 mM Hepes, 300 mM NaCl and 10 % Glycerol at pH 7.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Co-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.12(3)	5(2)	4(5)	0.3679	1315.864	78.335	3
3N/O	2.12(3)	8(2)	3(3)	0.2650	947.901	56.430	3
4N/O	2.11(2)	10(2)	2(3)	0.2148	768.246	45.735	3
5N/O	2.11(2)	12(2)	1(2)	0.1960	701.006	41.732	3
6N/O	2.10(2)	14(2)	0(2)	0.1958	700.433	41.698	3
7N/O	2.10(2)	16(2)	neg1(2)	0.2064	738.196	43.946	3

Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.23(4)	10(2)	neg14(6)	0.3553	1270.873	75.657	3
3S	2.23(3)	12(2)	neg15(5)	0.2778	993.752	59.159	3
4S	2.23(3)	15(2)	neg16(4)	0.2371	847.906	50.477	3
5S	2.23(3)	17(2)	neg16(4)	0.2159	772.246	45.973	3

6S	2.23(3)	19(2)	neg17(4)	0.2060	736.911	43.869	3
7S	2.23(3)	21(2)	neg17(4)	0.2029	725.801	43.208	3

Co-N(2.0) Co-N(2.2)

	r(Å)	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.03(2)	2(1)					
1N/O	2.18(2)	3(1)	0(2)	0.1651	590.442	39.900	5
2N/O	2.01(2)	2(1)					
2N/O	2.16(2)	1(1)	neg1(2)	0.1464	523.743	35.393	5
3N/O	2.04(2)	5(2)					
1N/O	2.18(2)	1(1)	neg1(2)	0.1497	535.611	36.195	5
4N/O	2.05(2)	8(2)					
1N/O	2.18(2)	0(2)	neg2(2)	0.1575	563.252	38.063	5
3N/O	2.02(2)	6(2)					
2N/O	2.17(2)	2(2)	neg2(2)	0.1605	574.098	38.796	5
5N/O	2.05(2)	11(2)					
1N/O	2.18(3)	1(2)	neg2(2)	0.1758	628.939	42.502	5
4N/O	2.02(3)	9(3)					
2N/O	2.17(3)	4(2)	neg3(2)	0.1840	658.303	44.486	5
3N/O	2.00(3)	7(3)					
3N/O	2.16(3)	6(3)	neg3(2)	0.1908	682.310	46.109	5
6N/O	2.05(3)	14(3)					
1N/O	2.17(3)	2(3)	neg3(3)	0.1974	706.075	47.715	5
5N/O	2.03(4)	14(5)					
2N/O	2.16(4)	6(4)	neg3(3)	0.2075	742.137	50.152	5
4N/O	2.07(0.19)	22(15)					
3N/O	2.11(7)	12(6)	neg2(4)	0.2117	757.158	51.167	5

Co-S(2.2) Co-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.14(3)	7(2)					
1S	2.28(3)	3(2)	neg20(5)	0.2372	848.408	57.333	5
2S	2.12(3)	8(3)					
2S	2.27(3)	6(2)	neg20(5)	0.2100	751.210	50.765	5
3S	2.26(4)	14(2)					
1S	1.70(9)	23(9)	neg11(6)	0.2323	830.924	56.152	5

4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.14(4)	12(3)					
2S	2.28(4)	8(3)	neg19(5)	0.2039	729.400	49.291	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.24(2)	15(2)					
2S	3.05(4)	12(5)	neg14(3)	0.1766	631.596	42.682	5
3S	2.14(6)	14(5)					
3S	2.28(5)	12(6)	neg19(5)	0.2024	724.003	48.926	5
6S	2.24(2)	19(2)					
1S	3.03(3)	5(3)	neg15(3)	0.1475	527.428	35.642	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.22(4)	16(5)					
3S	2.35(0.18)	27(25)	neg14(6)	0.1995	713.457	48.214	5

Co-N(2.0) Co-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	5(2)					5
1S	2.29(3)	4(2)	neg9(4)	0.2062	737.537	49.841	
1N/O	1.95(3)	2(2)					5
2S	2.26(3)	8(2)	neg12(4)	0.2052	733.862	49.592	
2N/O	1.98(4)	7(3)					
2S	2.28(3)	10(2)	neg11(4)	0.1921	687.118	46.434	5
3N/O	2.02(3)	9(2)					
1S	2.30(3)	6(2)	neg7(4)	0.1879	671.958	45.409	5
1N/O	2.56(0.11)	6(9)					
3S	2.21(4)	12(2)	neg17(6)	0.2530	904.872	61.149	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.04(4)	12(3)					
1S	2.31(3)	8(3)	neg6(4)	0.1827	653.323	44.150	5
2N/O	1.98(5)	9(4)	neg11(5)	0.1936	692.308	46.784	5

3S	2.28(4)	14(3)					
3N/O	2.01(5)	11(3)					
2S	2.29(4)	12(3)	neg9(5)	0.1901	679.925	45.948	5
5N/O	2.13(2)	12(2)					
1S	2.75(4)	11(6)	3(2)	0.1683	602.070	40.686	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.04(7)	14(4)					
2S	2.30(4)	14(6)	neg7(5)	0.1900	679.584	45.925	5
2N/O	1.35(0.18)	32(27)					
4S	2.24(4)	15(2)	neg14(6)	0.2277	814.501	55.042	5
3N/O	2.01(7)	13(5)					
3S	2.28(5)	16(5)	neg10(6)	0.1943	695.102	46.973	5
6N/O							
1S			No Fit	No Fit	No Fit	No Fit	5
1N/O	1.37(0.31)	30(50)					
6S	2.23(4)	19(2)	neg16(5)	0.2050	733.225	49.549	5
5N/O	2.07(7)	17(6)					
2S	2.29(4)	17(9)	neg6(6)	0.1897	678.541	45.854	5
2N/O	2.80(9)	13(14)					
5S	2.25(3)	17(2)	neg13(4)	0.1995	713.670	48.228	5
4N/O	2.05(7)	16(7)					
3S	2.29(5)	19(8)	neg8(6)	0.1941	694.153	46.909	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Co-N(2.0) Co-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.10(3)	15(4)					
1Imd	2.10(7)	9(9)	0(2)	0.1530	652.020	44.062	5
4N/O	2.10(2)	16(3)					
1Imd	2.00(1)	0(1)					
1Imd	2.16(1)	1(1)	neg1(1)	0.0612	218.858	17.101	7
3N/O							
1Imd			No Fit	No Fit	No Fit	No Fit	9

1Imd							
1Imd							
2N/O	2.10(2)	7(3)					
1Imd	1.90(8)	6(15)					
1Imd	2.10(6)	5(8)					
1Imd	2.22(5)	2(8)					
1Imd	1.98(5)	4(7)	neg2(2)	0.0511	185.665	20.763	11
1N/O	2.10(3)	2(4)					
1Imd	1.91(5)	2(11)					
1Imd	2.12(4)	9(8)					
1Imd	2.00(4)	8(9)					
1Imd	1.93(0.43)	44(190)					
1Imd	2.24(4)	6(7)	neg2(3)	0.0552	197.590	29.067	13
4N/O	2.10(3)	12(4)					
1Imd	2.11(7)	10(10)	1(2)	0.1579	564.691	38.160	5
3N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7
2N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.10(3)	2(3)					
1Imd	2.00(4)	7(6)					
1Imd	2.24(3)	5(5)					
1Imd	2.12(3)	8(6)					
1Imd	1.91(5)	1(8)	neg2(2)	0.0561	200.512	22.791	11
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
3N/O	2.12(2)	5(2)					
1Imd	1.97(2)	1(2)	neg2(2)	0.1810	647.412	43.750	5
2N/O	2.10(2)	7(3)					
1Imd	2.16(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0695	248.452	19.414	7
1N/O	2.10(3)	2(3)					
1Imd	1.96(2)	2(2)	neg1(2)	0.0684	244.587	22.651	9

1Imd	2.21(2)	3(4)					
1Imd	2.09(3)	4(4)					
0N/O							
1Imd	2.24(2)	8(4)					
1Imd	2.02(3)	11(4)					
1Imd	1.92(3)	5(4)					
1Imd	2.13(2)	11(4)	neg1(2)	0.1160	415.012	38.435	9
2N/O	2.12(2)	2(2)					
1Imd	1.98(2)	1(2)	neg2(3)	0.2309	825.767	55.803	5
1N/O	2.09(3)	2(3)					
1Imd	2.00(2)	1(1)					
1Imd	2.16(2)	2(1)	0(2)	0.1158	414.252	32.369	7
0N/O							
1Imd	1.97(2)	4(3)					
1Imd	2.08(2)	7(3)					
1Imd	2.20(2)	5(3)	neg1(2)	0.1548	553.624	43.259	7

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(6)	17(6)					
1S	2.30(2)	7(3)					
1Imd	1.99(3)	5(3)	neg5(3)	0.1224	521.452	40.745	7
3N/O	2.10(3)	13(6)					
1S	2.34(0.11)	28(24)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg2(1)	0.0541	193.602	17.930	9
2N/O	2.10(4)	9(4)					
1S	2.35(7)	20(15)					
1Imd	1.99(3)	0(3)					
1Imd	2.15(3)	1(3)					
1Imd	1.95(0.15)	12(20)	neg3(3)	0.0467	166.957	18.977	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(6)	17(6)					
1S	2.30(2)	8(3)					
1Imd	1.99(3)	5(3)	neg5(3)	0.1243	444.684	34.747	7
3N/O	2.10(3)	13(5)					
1S	2.37(0.14)	34(30)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0542	193.790	17.947	9

1Imd	1.99(2)	0(1)					
2N/O	2.10(4)	8(4)					
1S	2.36(7)	21(16)					
1Imd	1.99(4)	0(3)					
1Imd	1.95(0.15)	12(20)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0465	166.433	18.917	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(6)	16(6)					
1S	2.30(3)	8(3)					
1Imd	1.98(3)	5(3)	neg5(3)	0.1261	450.926	35.234	7
3N/O	2.10(3)	14(4)					
1S	2.40(0.16)	38(34)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0539	192.955	17.870	9
2N/O	2.10(3)	8(4)					
1S	2.37(7)	23(17)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	0(3)					
1Imd	1.96(0.15)	12(21)	neg3(2)	0.0463	165.550	18.817	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(5)	16(6)					
1S	2.30(3)	8(3)					
1Imd	1.98(4)	5(3)	neg6(4)	0.1275	455.928	35.625	7
3N/O	2.10(3)	12(4)					
1S	2.42(0.17)	40(36)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0535	191.411	17.727	9
2N/O	2.10(3)	8(4)					
1S	2.38(8)	25(19)					
1Imd	1.99(4)	0(3)					
1Imd	2.15(3)	1(3)					
1Imd	1.97(0.16)	12(22)	neg3(2)	0.046	164.505	18.698	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(2)	10(2)					
1S	2.75(4)	12(5)	2(2)	0.1317	470.965	36.800	7

1Imd	2.20(3)	3(3)					
3N/O	2.10(3)	12(4)					
1S	2.44(0.18)	42(36)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0532	190.416	17.635	9
2N/O	2.10(3)	8(4)					
1S	2.39(8)	27(20)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	0(3)					
1Imd	1.97(0.16)	12(22)	neg3(2)	0.0458	163.648	18.601	11

Co-N(2.0) Co-S(2.2) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	8(4)					
2S	2.29(4)	18(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.1236	441.935	34.532	7
2N/O	2.10(3)	8(4)					
2S	2.38(8)	33(12)					
1Imd	1.98(2)	0(1)					
1Imd	2.15(2)	1(1)	neg2(1)	0.0515	184.369	17.075	9
1N/O	2.09(3)	3(3)					
2S	2.38(5)	26(11)					
1Imd	2.16(4)	1(3)					
1Imd	2.00(0.11)	1(5)					
1Imd	1.98(0.19)	7(23)	neg3(2)	0.0435	155.489	17.673	11

Co-N(2.0) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	7(4)					
2S	2.29(4)	19(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.124	443.355	34.643	7
2N/O	2.10(3)	8(4)					
2S	2.40(8)	36(13)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg2(1)	0.0517	184.762	17.111	9
1N/O	2.09(3)	3(3)					
2S	2.39(5)	28(11)					
1Imd	2.17(4)	1(3)					
1Imd	2.01(0.18)	1(6)					
1Imd	1.98(0.24)	5(27)	neg3(2)	0.0434	155.224	17.643	11

Co-N(2.0) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	7(3)					
2S	2.30(4)	19(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.1245	445.292	34.794	7
2N/O	2.10(3)	8(3)					
2S	2.42(8)	37(14)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg2(1)	0.0514	183.787	17.021	9
1N/O	2.09(3)	3(3)					
2S	2.40(5)	30(11)					
1Imd	2.02(0.31)	1(10)					
1Imd	2.17(4)	1(3)					
1Imd	1.97(0.34)	4(34)	neg3(2)	0.0431	154.186	17.525	11

Co-N(2.0) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(3)	7(3)					
2S	2.30(4)	20(8)					
1Imd	1.96(2)	2(2)	neg6(3)	0.1248	446.571	34.894	7
2N/O	2.09(3)	8(3)					
2S	2.43(8)	39(14)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg2(1)	0.0509	182.057	16.860	9
1N/O	2.09(3)	3(3)					
2S	2.41(6)	31(12)					
1Imd	2.03(0.27)	1(19)					
1Imd	1.97(0.28)	3(27)					
1Imd	2.17(3)	1(4)	neg3(2)	0.0427	152.804	17.368	11

Co-N(2.0) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	6(2)					
2S	2.71(8)	29(13)					
1Imd	2.20(2)	1(2)	3(2)	0.1557	556.990	43.522	7
2N/O	2.09(3)	8(3)					
2S	2.44(9)	40(15)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg2(1)	0.0506	181.153	16.777	9
1N/O	2.09(3)	3(3)					
2S	2.41(6)	32(12)					
1Imd	2.17(3)	1(4)					
1Imd	2.04(0.17)	1(18)	neg3(2)	0.0424	151.705	17.243	11

1Imd	1.96(0.18)	2(19)					

Co-N(2.0) Co-S(2.2) Co-S(2.3) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	19(10)					
1S	2.44(6)	9(7)					
1S	2.27(3)	4(3)					
1Imd	1.98(3)	3(2)	neg6(3)	0.105	375.635	34.788	9
2N/O	2.07(3)	9(4)					
1S	2.66(6)	13(6)					
1S	2.41(5)	11(5)					
1Imd	2.15(2)	1(1)					
1Imd	2.00(2)	0(1)	neg1(1)	0.0421	150.622	17.120	11
1N/O	2.07(3)	3(4)					
1S	2.35(4)	9(6)					
1S	2.58(0.10)	19(14)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	0(3)					
1Imd	1.96(0.16)	12(22)	neg3(2)	0.0372	133.034	19.570	11

Co-N(2.0) Co-S(2.2) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(7)	18(9)					
1S	2.44(6)	9(6)					
1S	2.28(3)	4(3)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1063	380.182	35.209	9
2N/O	2.07(3)	8(4)					
1S	2.66(6)	12(6)					
1S	2.42(5)	11(5)					
1Imd	2.00(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0412	147.497	16.765	11
1N/O	2.07(3)	3(4)					
1S	2.35(4)	9(6)					
1S	2.59(9)	19(13)					
1Imd	1.96(0.16)	13(23)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0362	129.416	19.038	11

Co-N(2.0) Co-S(2.2) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	21(10)					
1S	2.27(3)	4(2)	neg6(3)	0.1021	365.072	33.810	9

1S	2.44(7)	12(8)					
1Imd	1.98(2)	3(2)					
2N/O	2.07(3)	10(5)					
1S	2.37(5)	11(5)					
1S	2.65(7)	16(8)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.04	142.918	16.245	11
1N/O	2.07(3)	3(4)					
1S	2.35(4)	10(6)					
1S	2.59(9)	20(13)					
1Imd	1.97(0.16)	13(23)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0353	126.382	18.591	11

Co-N(2.0) Co-S(2.2) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	20(10)					
1S	2.27(3)	4(2)					
1S	2.44(7)	13(8)					
1Imd	1.98(2)	3(2)	neg6(3)	0.1014	362.644	33.585	9
2N/O	2.07(4)	11(5)					
1S	2.37(5)	12(5)					
1S	2.64(7)	17(8)					
1Imd	1.99(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0393	140.544	15.975	11
1N/O	2.07(4)	3(4)					
1S	2.35(4)	10(6)					
1S	2.59(9)	20(13)					
1Imd	1.97(0.17)	14(23)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0347	124.012	18.243	11

Co-N(2.0) Co-S(2.3) Co-S(2.4) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(7)	18(9)					
1S	2.44(7)	10(7)					
1S	2.28(3)	4(3)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1058	378.376	35.042	9
2N/O	2.07(3)	9(4)					
1S	2.39(5)	12(5)					
1S	2.66(6)	14(7)					
1Imd	2.15(2)	1(1)					
1Imd	2.00(2)	0(1)	neg1(1)	0.0397	142.076	16.149	11

1N/O	2.07(3)	3(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	18(11)					
1Imd	1.99(4)	1(2)					
1Imd	1.96(0.15)	12(21)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0353	126.205	18.565	11

Co-N(2.0) Co-S(2.3) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	19(10)					
1S	2.27(3)	5(2)					
1S	2.44(7)	12(8)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1031	368.639	34.140	9
2N/O	2.07(3)	10(4)					
1S	2.39(5)	12(5)					
1S	2.66(6)	14(7)					
1Imd	2.00(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.0389	139.157	15.817	11
1N/O	2.07(3)	3(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	18(11)					
1Imd	1.96(0.15)	12(21)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0344	123.084	18.106	11

Co-N(2.0) Co-S(2.3) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(8)	19(10)					
1S	2.27(3)	5(2)					
1S	2.45(7)	13(8)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1023	366.048	33.900	9
2N/O	2.07(3)	10(5)					
1S	2.38(5)	12(5)					
1S	2.65(6)	15(7)					
1Imd	2.15(2)	1(1)					
1Imd	1.99(2)	0(1)	neg1(1)	0.0383	136.859	15.556	11
1N/O	2.07(3)	3(3)					
1S	2.36(4)	10(6)					
1S	2.60(8)	19(11)					
1Imd	1.99(4)	0(2)					
1Imd	2.15(3)	1(3)					
1Imd	1.96(0.15)	13(21)	neg3(2)	0.0337	120.655	17.749	11

Co-N(2.0) Co-S(2.4) Co-S(2.5) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(7)	18(9)					
1S	2.28(3)	5(2)					
1S	2.45(7)	12(8)					
1Imd	1.98(3)	3(2)	neg6(3)	0.1042	372.641	34.511	9
2N/O	2.07(3)	9(4)					
1S	2.40(5)	12(5)					
1S	2.66(6)	13(6)					
1Imd	2.00(2)	0(1)					
1Imd	2.15(2)	1(1)	neg1(1)	0.038	135.944	15.452	11
1N/O	2.07(3)	3(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	17(10)					
1Imd	1.96(0.14)	12(20)					
1Imd	2.15(3)	1(3)					
1Imd	1.99(4)	1(2)	neg3(2)	0.0337	120.642	17.747	11

Co-N(2.0) Co-S(2.4) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	3N/O	2.07(7)	18(9)				
1S	1S	2.28(3)	5(2)				
1S	1S	2.45(7)	13(8)				
1Imd	1Imd	1.98(3)	3(2)	neg6(3)	0.1034	369.900	9
2N/O	2N/O	2.07(3)	10(4)				
1S	1S	2.39(5)	12(5)				
1S	1S	2.66(6)	14(6)				
1Imd	1Imd	2.00(2)	0(1)				
1Imd	1Imd	2.15(2)	1(1)	neg1(1)	0.0374	133.740	11
1N/O	1N/O	2.07(3)					
1S	2.36(4)	9(6)					
1S	2.60(8)	18(10)					
1Imd	2.15(3)	1(3)					
1Imd	1.96(0.14)	12(20)					
1Imd	1.99(4)	1(2)	3(3)	neg3(2)	0.033	118.171	11

Co-N(2.0) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(7)	18(9)					
1S	2.46(7)	12(7)					
1S	2.28(3)	5(3)					
1Imd	1.98(3)	3(2)	neg7(3)	0.1054	377.150	34.928	9

2N/O	2.07(3)	9(4)					
1S	2.40(5)	12(5)					
1S	2.67(5)	13(6)					
1Imd 0°	2.15(2)	1(1)					
1Imd 0°	2.00(2)	0(1)	neg1(1)	0.0365	130.623	14.847	11
2N/O	2.07(4)	11(5)					
1S	2.40(5)	12(5)					
1S	2.68(6)	14(6)					
1Imd 0°	2.15(2)	2(1)					
1Imd 5°	2.00(2)	1(1)	neg1(1)	0.0374	133.832	15.212	11
2N/O	2.02(7)	16(11)					
1S	2.51(8)	12(8)					
1S	2.32(4)	6(4)					
1Imd 0°	1.97(2)	3(2)					
1Imd 10°	2.09(4)	2(3)	neg5(2)	0.0613	219.089	24.903	11
2N/O	2.03(8)	17(12)					
1S	2.50(8)	14(10)					
1S	2.31(4)	7(5)					
1Imd 5°	1.97(2)	2(2)					
1Imd 10°	2.10(4)	2(2)	neg5(2)	0.0595	212.666	24.172	11
1N/O	2.07(3)	3(3)					
1S	2.37(4)	10(5)					
1S	2.61(7)	17(9)					
1Imd	1.96(0.14)	12(20)					
1Imd	1.99(4)	1(2)					
1Imd	2.15(3)	1(3)	neg3(2)	0.0326	116.576	17.149	13

Co-N(2.2) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(8)	19(10)					
1S	2.45(8)	13(9)					
1S	2.28(3)	5(3)					
1Imd	1.98(3)	3(2)	neg7(3)	0.1041	372.421	34.490	9
2N/O	2.08(3)	10(4)					
1S	2.41(5)	13(5)					
1S	2.68(5)	12(5)					
1Imd 0°	2.15(2)	1(1)					
1Imd 0°	1.99(2)	0(1)	neg2(1)	0.0356	127.368	14.477	11
2N/O	2.08(4)	12(5)					
1S	2.41(6)	14(6)					
1S	2.69(6)	13(6)					
1Imd 0°	2.15(2)	1(1)					
1Imd 5°	2.00(2)	1(1)	neg1(1)	0.0371	132.615	15.074	11

2N/O	2.04(9)	19(14)					
1S	2.51(9)	13(9)					
1S	2.31(4)	6(5)					
1Imd 0°	1.97(2)	3(2)					
1Imd 10°	2.09(4)	2(3)	neg6(2)	0.0621	221.978	25.231	11
2N/O	2.05(9)	20(14)					
1S	2.50(9)	15(11)					
1S	2.31(4)	7(5)					
1Imd 5°	1.97(2)	2(2)					
1Imd 10°	2.10(4)	2(2)	neg5(3)	0.0602	215.435	24.487	11
1N/O	2.08(3)	3(3)					
1S	2.38(4)	10(6)					
1S	2.63(7)	16(8)					
1Imd	1.99(3)	1(2)					
1Imd	1.98(0.18)	15(24)					
1Imd	2.15(3)	1(2)	neg3(2)	0.0323	115.496	16.990	13

Co-N(2.0) Co-N(2.2) Co-S(2.5) Co-S(2.6) Co-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(5)	5(6)					
1N/O	2.11(3)	0(3)					
1S	2.66(5)	8(4)					
1S	2.42(4)	8(4)					
1Imd 0°	2.00(2)	2(2)					
1Imd 0°	2.15(2)	2(1)	neg2(2)	0.0259	92.765	13.646	13
1N/O	1.95(4)	3(5)					
1N/O	2.12(2)	1(3)					
1S	2.43(4)	9(4)					
1S	2.68(5)	10(4)					
1Imd 0°	2.16(2)	1(1)					
1Imd 5°	2.01(2)	2(2)	neg2(2)	0.0264	94.424	13.890	13
1N/O	1.97(2)	1(1)					
1N/O	2.15(3)	0(3)					
1S	2.74(6)	10(6)					
1S	2.47(7)	15(7)					
1Imd 0°	2.15(6)	9(8)					
1Imd 10°	2.10(3)	2(3)	0(2)	0.0349	124.764	18.353	13
1N/O	1.97(2)	1(1)					
1N/O	2.15(3)	0(3)					
1S	2.74(6)	11(6)					
1S	2.46(7)	15(7)					
1Imd 5°	2.15(6)	8(8)					
1Imd 10°	2.10(3)	2(3)	0(2)	0.0362	129.633	19.070	13

APPENDIX H

ADDITIONAL FIT TABLES FOR WT NiSOD

Table H.1. Additional Fits for Reduced WT NiSOD in Buffer with 50 mM Tris, 100 mM NaCl and 10 % Glycerol at pH 8.0.

Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

	Ni-N(2.0)						
N	**r(Å)**	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(2)	0(1)	19(3)	0.3545	3581.114	182.341	3
3N/O	2.07(1)	2(1)	16(2)	0.3138	3170.650	161.441	3
4N/O	2.06(2)	3(1)	14(2)	0.3182	3214.425	163.670	3
5N/O	2.04(2)	5(1)	12(2)	0.3468	3503.704	178.400	3
6N/O	2.03(2)	7(2)	10(2)	0.3889	3929.498	200.080	3
7N/O	2.02(2)	9(2)	9(3)	0.4371	4416.304	224.867	3

	Ni-S(2.2)						
N	**r(Å)**	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.17(1)	3(1)	0(3)	0.1645	1661.475	84.598	3
3S	2.17(1)	5(1)	neg2(2)	0.1410	1424.098	72.511	3
4S	2.16(1)	7(1)	neg4(2)	0.1570	1586.289	80.770	3
5S	2.15(1)	9(1)	neg5(3)	0.1891	1910.979	97.302	3
6S	2.15(2)	11(1)	neg6(3)	0.2272	2295.713	116.892	3
7S	2.14(2)	13(1)	neg7(3)	0.2667	2694.052	137.174	3

	Ni-N(2.0) Ni-N(2.2)						
N	**r(Å)**	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.06(2)	1(1)					
1N/O	2.41(2)	3(2)	16(4)	0.2822	2850.881	161.618	5
2N/O	2.08(1)	0(1)					
2N/O	2.51(7)	9(10)	20(3)	0.3040	3071.272	174.112	5
3N/O	2.06(1)	1(1)					
1N/O	2.40(2)	2(2)	14(2)	0.2181	2203.474	124.916	5
4N/O							
1N/O			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.07(1)	1(1)					
2N/O	2.47(4)	6(5)	18(2)	0.2333	2356.986	133.619	5
5N/O	2.04(2)	5(2)					
1N/O	3.93(8)	2(6)	12(2)	0.3341	3375.445	191.356	5
4N/O	2.05(1)	3(1)	14(2)	0.2040	2061.384	116.861	5

2N/O	2.41(2)	2(2)					
3N/O	2.07(1)	1(1)					
3N/O	2.50(5)	11(7)	18(2)	0.2317	2340.957	132.710	5
6N/O	2.03(2)	7(1)					
1N/O	2.37(2)	3(1)	9(2)	0.2251	2274.074	128.918	5
5N/O	2.04(1)	5(1)					
2N/O	2.40(2)	1(2)	12(2)	0.2000	2020.583	114.548	5
4N/O	2.06(1)	3(1)					
3N/O	2.47(3)	8(5)	16(2)	0.2055	2075.997	117.689	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.16(1)	0(1)					
1S	2.03(1)	1(1)	neg8(2)	0.0689	696.352	39.477	5
2S	2.17(1)	1(1)					
2S	2.04(1)	4(1)	neg10(2)	0.0659	665.434	37.724	5
3S	2.15(1)	3(0)					
1S	2.00(1)	1(1)	neg9(2)	0.0662	668.772	37.913	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.16(1)	3(1)					
2S	2.01(1)	5(1)	neg11(2)	0.0841	849.329	48.149	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.17(1)	7(1)					
2S	2.48(3)	12(4)	neg1(3)	0.1119	1130.519	64.090	5
3S	2.16(1)	3(1)					
3S	2.02(2)	8(2)	neg12(2)	0.1117	1128.149	63.955	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.17(1)	9(1)					
2S	2.47(2)	9(3)	neg3(3)	0.1140	1151.481	65.278	5
4S	2.17(2)	7(1)					
3S	1.74(9)	50(27)	neg1(4)	0.1475	1490.025	84.470	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.94(2)	2(1)					5
1S	2.19(1)	1(0)	2(2)	0.0692	699.314	39.644	
1N/O	1.89(1)	0(1)					5
2S	2.17(1)	2(0)	neg2(2)	0.0608	614.055	34.811	
2N/O	1.90(2)	4(1)					
2S	2.17(1)	2(0)	neg2(2)	0.0712	719.246	40.774	5
3N/O	1.95(2)	5(1)					
1S	2.19(1)	0(0)	3(2)	0.0651	657.846	37.294	5
1N/O	1.86(1)	0(1)					
3S	2.16(1)	5(0)	neg4(2)	0.0830	838.802	47.552	5
1N/O	2.32(1)	3(1)					
4S	2.14(2)	10(1)	neg8(3)	0.0864	872.804	49.480	5
4N/O	1.97(2)	9(2)					
1S	2.19(1)	0(1)	4(2)	0.0763	770.907	43.703	5
2N/O	2.02(0.11)	20(27)					
3S	2.17(2)	6(1)	0(4)	0.1267	1279.817	72.533	5
3N/O	1.93(4)	9(3)					
2S	2.18(1)	3(1)	0(3)	0.0947	956.766	54.239	5
5N/O	1.99(4)	12(2)					
1S	2.19(1)	0(1)	5(3)	0.0919	928.069	52.613	5
1N/O	2.82(5)	1(4)					
5S	2.16(2)	9(1)	neg5(3)	0.1703	1720.328	97.526	5
4N/O	2.04(7)	17(10)					
2S	2.19(1)	3(1)	6(5)	0.0964	973.616	55.195	5
2N/O	2.31(1)	1(1)					
4S	2.13(2)	11(1)	neg11(3)	0.0803	810.793	45.964	5
3N/O	2.06(7)	23(32)					
3S	2.18(2)	5(1)	2(6)	0.1218	1230.955	69.783	5
6N/O	2.01(5)	16(3)					
1S	2.19(1)	0(1)	6(4)	0.1075	1085.610	61.544	5
1N/O	1.58(4)	6(4)					
6S	2.14(2)	11(1)	neg7(3)	0.2113	2134.306	120.995	5

5N/O	2.08(5)	19(10)					
2S	2.19(1)	3(1)	7(5)	0.0929	938.854	53.224	5
2N/O	2.31(1)	1(1)					
5S	2.14(2)	13(1)	neg10(3)	0.0799	807.726	45.790	5
4N/O	2.09(5)	21(29)					
3S	2.18(2)	5(1)	4(7)	0.1162	1173.947	66.552	5
3N/O	2.14(0.23)	20(50)					
4S	2.17(2)	7(1)	0(10)	0.1425	1440.141	81.642	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.04(2)	3(1)					
1Imd	1.88(2)	1(2)	8(2)	0.3023	3038.694	172.265	5
4N/O	2.03(2)	4(2)					
1Imd	1.89(3)	1(2)					
1Imd	2.06(4)	1(3)	9(2)	0.2423	2447.557	156.497	7
3N/O	2.04(2)	2(2)					
1Imd	1.60(8)	16(14)					
1Imd	1.90(2)	2(2)					
1Imd	2.06(4)	1(3)	11(2)	0.1704	1721.138	126.186	9
2N/O	2.05(2)	0(2)					
1Imd	1.86(2)	6(2)					
1Imd	1.64(0.10)	16(16)					
1Imd	2.09(3)	7(2)					
1Imd	1.97(3)	8(3)	9(2)	0.1491	1506.246	129.406	11
1N/O	2.06(2)	3(2)					
1Imd	1.98(2)	10(3)					
1Imd	2.10(2)	9(3)					
1Imd	1.87(2)	7(3)					
1Imd	1.47(0.17)	14(21)					
1Imd	1.71(0.20)	9(19)	10(3)	0.1451	1466.053	152.086	13
4N/O	2.05(1)	1(1)					
1Imd	1.89(2)	1(2)	9(2)	0.2616	2642.781	149.821	5
3N/O	2.08(1)	1(1)					
1Imd	2.41(2)	0(2)					
1Imd	1.61(2)	5(3)	20(2)	0.1824	1842.408	117.804	7
2N/O	2.05(2)	0(2)					
1Imd	2.09(3)	5(3)					
1Imd	1.87(3)	4(4)	9(2)	0.1837	1856.096	136.081	9

1Imd	1.97(4)	6(5)					
1N/O	2.06(2)	3(2)					
1Imd	1.87(2)	7(2)					
1Imd	1.98(2)	9(2)					
1Imd	2.10(2)	8(2)					
1Imd	1.61(0.14)	22(24)	10(2)	0.1460	1475.386	126.755	11
0N/O							
1Imd	2.00(2)	11(2)					
1Imd	1.81(0.23)	14(49)					
1Imd	2.12(2)	10(2)					
1Imd	1.89(2)	8(2)					
1Imd	1.50(0.16)	14(16)	9(3)	0.2297	2320.879	199.394	11
3N/O	2.06(1)	0(1)					
1Imd	1.92(2)	1(2)	11(2)	0.2451	2476.412	140.389	5
2N/O	2.05(2)	0(1)					
1Imd	1.92(2)	3(1)					
1Imd	2.06(3)	2(2)	11(2)	0.1766	1784.666	114.112	7
1N/O	2.06(2)	3(2)					
1Imd	2.10(3)	5(4)					
1Imd	1.98(6)	5(8)					
1Imd	1.90(6)	2(10)	10(2)	0.1810	1829.035	134.097	9
0N/O							
1Imd	1.90(1)	8(1)					
1Imd	2.12(1)	10(1)					
1Imd	2.01(1)	11(1)					
1Imd	1.54(0.12)	23(24)	11(0)	0.2282	2305.350	169.018	9
2N/O	2.07(1)	2(1)					
1Imd	1.95(2)	1(2)	13(2)	0.2706	2733.930	154.988	5
1N/O	2.07(2)	3(1)					
1Imd	2.08(2)	4(1)					
1Imd	1.94(2)	4(1)	12(2)	0.1946	1965.575	125.679	7
0N/O							
1Imd	2.00((1)	11(1)					
1Imd	1.89(1)	8(1)					
1Imd	2.12(1)	10(1)	10(2)	0.2393	2418.030	154.609	7

Ni-N(2.0) Ni-S(2.0)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O							
2S			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-S(2.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(2)	4(1)					
2S	2.17(1)	2(0)	neg1(2)	0.071	717.800	40.692	5

Ni-N(2.2) Ni-S(2.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(2)	4(1)					
2S	2.17(1)	2(0)	neg2(2)	0.0785	793.545	44.986	5

Ni-N(2.0) Ni-N(2.2) Ni-S(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(3)	3(2)					
1N/O	2.89(4)	0(4)					
2S	2.15(2)	2(2)	3(4)	0.1467	1482.026	94.761	7

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(2)	0(1)					
1N/O	2.13(0.33)	24(202)					
2S	2.17(2)	2(0)	0(10)	0.096	602.383	38.516	7

Ni-N(2.0) Ni-N(2.2) Ni-S(2.0) Ni-S(2.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	3(3)					
1N/O	2.22(0.21)	0(40)					
1S	2.10(2)	4(4)					
1S	2.22(2)	5(6)	neg2(6)	0.0445	449.128	32.928	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.29(6)	7(3)					
1S	2.12(2)	5(1)					
1S	2.25(3)	6(3)	neg2(3)	0.0406	410.532	30.098	9

Ni-N(1.8) Ni-N(2.2) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	6(1)					
1N/O	1.97(1)	8(2)					
1S	2.20(1)	3(1)					
1S	1.98(7)	13(18)	0(3)	0.0406	410.320	30.083	9

Ni-N(1.9) Ni-N(2.2) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.86(2)	3(1)					
1N/O	2.31(6)	6(3)					
1S	2.12(2)	4(1)					
1S	2.26(3)	4(3)	neg3(3)	0.0396	399.638	29.300	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	3(2)					
1N/O	2.17(0.30)	4(58)					
1S	2.22(3)	4(3)					
1S	2.10(2)	4(4)	neg3(7)	0.0462	466.577	34.207	9

Ni-N(1.9) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	3(1)					
1N/O	2.30(6)	6(3)					
1S	2.12(2)	5(1)					
1S	2.26(3)	5(3)	neg2(3)	0.0405	409.617	30.031	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	2(2)					
1N/O	2.19(5)	6(2)					
1S	2.10(3)	3(3)					
1S	2.20(3)	5(3)	neg4(3)	0.0375	376.759	27.622	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	2(1)					
1N/O	2.19(5)	7(3)					
1S	2.11(3)	3(4)					
1S	2.20(4)	5(4)	neg3(3)	0.039	394.455	28.920	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	2(2)					
1N/O	2.19(4)	7(2)					
1S	2.11(3)	3(3)					
1S	2.20(3)	5(3)	neg4(3)	0.0373	376.451	27.600	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(2)					
1N/O	2.21(4)	7(4)					
1S	2.10(2)	4(2)					
1S	2.21(3)	6(3)					
1C	2.87(4)	1(4)	neg4(2)	0.0276	278.696	23.944	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.20(6)	6(3)					
1S	2.11(2)	4(2)					
1S	2.21(3)	5(3)					
2C	2.89(4)	6(5)		0.0277	279.936	24.050	11

Ni-N(1.9) Ni-N(2.2) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.31(6)	6(3)					
1S	2.12(1)	4(1)					
1S	2.26(3)	5(2)					
2C	2.90(4)	6(4)	neg3(2)	0.0278	281.341	24.171	11

Ni-N(1.9) Ni-N(2.2) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.31(5)	6(2)					
1S	2.12(1)	4(1)					
1S	2.26(3)	5(2)					
3C	2.91(4)	10(6)	neg2(2)	0.0289	292.140	25.100	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(1)	3(1)					
1N/O	2.33(2)	9(1)					
1S	2.29(2)	7(1)					
1S	2.15(1)	6(1)					
1Imd	1.92(4)	5(4)	1(2)	0.0232	234.767	20.170	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.7)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	4(1)					
1N/O	2.28(4)	9(2)					
1S	2.12(2)	6(1)					
1S	2.25(3)	8(2)					
1C	2.91(3)	0(3)	neg2(2)	0.0304	306.810	26.359	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.7)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.29(5)	7(3)					
1S	2.12(1)	5(1)					
1S	2.26(3)	6(2)					
2C	2.90(4)	6(5)	neg2(2)	0.0298	300.605	25.826	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	4(1)					
1N/O	2.28(4)	9(3)					
1S	2.12(2)	6(1)					
1S	2.25(3)	7(2)					
1C	2.91(4)	0(4)	neg2(2)	0.0304	307.371	26.407	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.29(5)	7(3)					
1S	2.12(1)	5(1)					
1S	2.25(3)	6(2)					
2C	2.90(4)	6(5)	neg2(2)	0.0299	301.753	25.925	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	4(1)					
1N/O	2.28(4)	9(3)					
1S	2.12(2)	6(1)					
1S	2.25(3)	7(2)					
1C	2.91(4)	0(4)	neg2(2)	0.0305	307.967	26.458	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.29(5)	7(3)					
1S	2.12(1)	5(1)					
1S	2.25(3)	6(2)					
2C	2.90(4)	6(5)	neg2(2)	0.03	303.093	26.040	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(1)	5(1)					
1N/O	2.30(2)	10(1)					
1S	2.27(2)	8(1)					
1S	2.13(1)	7(1)					
1C	2.92(4)	3(5)	0(2)	0.0255	257.938	22.160	11

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(1)	5(1)					
1N/O	2.30(2)	10(1)					
1S	2.27(2)	8(1)	neg1(2)	0.0244	246.945	21.216	11

1S	2.13(1)	7(1)					
2C	2.92(4)	8(6)					

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-C(3.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	4(1)					
1N/O	2.29(5)	8(3)					
1S	2.12(2)	5(1)					
1S	2.26(3)	6(2)					
2C	2.91(5)	6(5)					
2C	3.28(0.22)	26(48)	neg1(2)	0.0287	289.579	30.040	13

Ni-N(2.0) Ni-N(2.2) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-C(3.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	4(1)					
1N/O	2.29(5)	8(3)					
1S	2.12(2)	5(1)					
1S	2.26(3)	6(2)					
2C	2.91(5)	6(5)					
2C	3.29(0.20)	25(44)	neg1(2)	0.0286	289.102	29.991	13

Ni-N(1.9) Ni-N(2.2) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9) Ni-C(3.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.31(5)	6(3)					
1S	2.12(1)	5(1)					
1S	2.26(3)	5(2)					
2C	2.91(4)	6(5)					
2C	3.26(0.24)	30(55)	neg2(2)	0.0268	270.682	28.080	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(1)					
1N/O	2.20(6)	6(4)					
1S	2.11(1)	4(2)					
1S	2.21(3)	5(3)					
2C	2.89(4)	6(5)					
1Cl	3.51(4)	7(5)	neg3(2)	0.022	222.099	23.040	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	2(1)					
1N/O	2.19(6)	6(3)					
1S	2.11(2)	3(3)					
1S	2.20(4)	4(3)					
2C	2.90(5)	7(5)					
2Cl	3.51(5)	16(8)	neg3(2)	0.0247	249.491	25.882	13

Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.93(3)	5(4)					
1S	2.11(5)	6(10)					
1S	2.19(2)	0(1)					
2C	2.91(3)	4(3)					
1Cl	3.52(6)	9(7)					
1Cl	4.00(4)	5(4)	neg1(3)	0.0323	326.622	33.883	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(1)	0(1)					
1N/O	2.15(0.42)	36(129)					
2S	2.17(1)	2(0)					
2C	2.91(3)	3(3)					
1Cl	3.52(6)	9(7)					
1Cl	4.00(4)	4(4)	neg1(3)	0.0287	289.707	30.054	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-C(2.8) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(1)	0(1)					
1N/O	1.98(1.08)	67(200)					
2S	2.17(1)	2(0)					
2C	2.91(3)	3(3)					
1Cl	3.53(6)	10(8)					
1Cl	4.01(4)	4(4)	neg1(2)	0.0309	312.008	32.367	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(0.36)	31(132)					
1N/O	1.89(1)	0(1)					
2S	2.17(1)	2(0)					
2C	2.90(3)	3(3)					
1Cl	3.52(6)	9(7)					
1Cl	4.00(4)	4(4)	neg1(4)	0.0289	291.744	30.265	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.0) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	0(1)					
1N/O	2.37(2)	0(2)					
2S	2.15(1)	3(0)					
2C	2.89(3)	4(3)					
1Cl	3.50(6)	10(7)					
1Cl	3.98(3)	4(3)	neg4(2)	0.0247	249.696	25.903	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(1)	0(1)					
1N/O	2.19(0.62)	43(144)					
2S	2.17(1)	2(0)					
2C	2.91(3)	3(3)					
1Cl	3.53(7)	10(8)					
1Cl	4.01(4)	4(4)	neg1(3)	0.0309	312.270	32.394	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(1)	0(1)					
1N/O	2.15(0.42)	35(128)					
2S	2.17(1)	2(0)					
2C	2.91(3)	3(3)					
1Cl	3.52(6)	9(7)					
1Cl	4.00(4)	4(4)	neg1(3)	0.0287	289.639	30.047	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.0) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(1)	0(1)					
1N/O	2.02(1.16)	70(251)					
2S	2.17(1)	2(0)					
2C	2.91(3)	3(3)					
1Cl	3.54(7)	10(8)					
1Cl	4.02(4)	4(4)	0(2)	0.035	353.899	36.713	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.0) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1N/O							
2S							
2C							
1Cl							
1Cl			No Fit	No Fit	No Fit	No Fit	13

Ni-N(1.8) Ni-N(2.1) Ni-S(2.0) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(1)	0(1)					
1N/O	2.19(0.71)	63(281)					
2S	2.17(1)	2(0)					
2C	2.91(3)	3(3)					
1Cl	3.54(7)	10(8)					
1Cl	4.02(4)	4(4)	0(3)	0.0349	352.856	36.605	13

Ni-N(1.8) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.92(3)	5(3)					
1S	2.12(5)	5(8)					
1S	2.19(2)	0(1)					
2C	2.91(3)	4(3)					
1Cl	3.52(6)	9(7)					
1Cl	4.00(4)	4(4)	neg1(3)	0.0317	319.897	33.186	13

Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.93(3)	5(4)					
1S	2.11(5)	6(10)					
1S	2.19(2)	0(1)					
2C	2.91(3)	4(3)					
1Cl	3.52(6)	9(7)					
1Cl	4.00(4)	4(4)	neg1(3)	0.0323	326.712	33.893	13

Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.94(3)	5(6)					
1S	2.11(4)	6(12)					
1S	2.19(2)	0(1)					
2C	2.91(3)	4(3)					
1Cl	3.52(6)	9(7)					
1Cl	4.00(4)	4(4)	neg1(3)	0.0332	335.809	34.834	13

Ni-N(2.0) Ni-S(2.0) Ni-S(2.1) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.92(3)	5(4)					
1S	2.12(5)	5(8)					
1S	2.19(2)	0(1)					
2C	2.92(4)	4(4)					
1Cl	3.53(7)	9(8)					
1Cl	4.01(4)	4(4)	0(3)	0.0349	352.683	36.587	13

Ni-N(2.0) Ni-S(2.0) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.92(3)	5(4)					
1S	2.12(6)	6(9)					
1S	2.19(2)	0(1)					
2C	2.91(4)	4(3)					
1Cl	3.53(6)	9(7)					
1Cl	4.01(4)	4(4)	neg1(3)	0.033	333.268	34.573	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(1)					
1N/O	2.21(6)	6(4)					
1S	2.11(1)	4(1)					
1S	2.21(2)	5(2)					
2C	2.90(3)	6(3)					
1Cl	3.51(3)	8(4)					
1Cl	3.99(2)	4(2)	neg3(2)	0.0099	100.083	13.101	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.15(1)	7(1)					
1S	2.14(2)	4(1)					
1S	2.20(2)	0(3)					
2C	2.93(2)	5(3)					
1Cl	3.53(3)	9(4)					
1Cl	4.01(2)	3(2)	neg1(1)	0.0072	72.426	9.480	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.15(2)	7(1)					
1S	2.13(2)	5(1)					
1S	2.21(2)	0(3)					
1C	2.92(2)	0(2)					
1Cl	3.53(3)	8(4)					
1Cl	4.01(2)	3(2)	0(2)	0.0082	82.420	10.788	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(1)					
1N/O	2.21(6)	6(4)					
1S	2.11(1)	4(1)					
1S	2.21(2)	5(2)					
1C	2.90(3)	6(3)					
1Cl	3.51(3)	8(4)					
1Cl	3.99(2)	4(2)	neg3(2)	0.0099	99.771	13.060	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(1)					
1N/O	2.21(6)	6(4)					
1S	2.11(1)	4(1)					
1S	2.21(2)	5(2)					
1C	2.90(3)	6(3)					
1Cl	3.51(3)	8(4)	neg3(2)	0.0098	99.284	12.996	15

1Cl	3.99(2)	3(2)					

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(1)					
1N/O	2.22(4)	7(4)					
1S	2.11(1)	4(1)					
1S	2.22(2)	6(3)					
2C	2.89(3)	3(3)					
1C	3.09(6)	3(6)					
1Cl	3.51(4)	8(4)					
1Cl	3.99(2)	3(2)	neg3(2)	0.0078	79.021	14.012	17

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(2)					
1N/O	2.21(4)	7(3)					
1S	2.11(2)	4(2)					
1S	2.21(3)	5(3)					
1C	3.02(7)	4(10)					
1C	2.86(3)	1(3)					
1Cl	3.51(4)	8(4)					
1Cl	3.99(3)	3(2)	neg3(2)	0.0076	77.267	13.701	17

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(2)					
1N/O	2.21(4)	7(3)					
1S	2.11(2)	4(2)					
1S	2.21(3)	5(3)					
1C	3.02(7)	4(10)					
1C	2.86(3)	1(3)					
1Cl	3.51(4)	8(4)					
1Cl	3.99(3)	3(2)	neg3(2)	0.0076	77.267	13.701	17

Table H.2. Additional Fits for As Isolated WT NiSOD in Buffer with 50 mM Tris, 100 mM NaCl and 10 % Glycerol at pH 8.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Ni-N(2.0)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(1)	0(1)	16(3)	0.2818	2700.974	137.527	3
3N/O	2.07(1)	2(1)	14(2)	0.2510	2406.345	122.525	3

4N/O	2.06(1)	4(1)	12(2)	0.2756	2641.988	134.523	3
5N/O	2.05(2)	6(1)	11(2)	0.3260	3124.548	159.094	3
6N/O	2.04(2)	8(2)	9(2)	0.3864	3704.076	188.602	3
7N/O	2.03(3)	10(2)	7(3)	0.4402	4219.088	214.825	3

Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.17(1)	3(1)	neg3(3)	0.1470	1409.409	71.763	3
3S	2.17(1)	6(1)	neg4(2)	0.1455	1395.043	71.032	3
4S	2.16(1)	8(1)	neg6(3)	0.1773	1699.493	86.534	3
5S	2.16(2)	11(1)	neg7(3)	0.2181	2090.757	106.456	3
6S	2.15(2)	13(1)	neg8(3)	0.2594	2486.298	126.596	3
7S	2.15(2)	15(2)	neg9(3)	0.2983	2859.660	145.606	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.08(1)	0(1)					
1N/O	2.46(4)	2(4)	16(3)	0.2266	2172.509	123.161	5
2N/O	2.08(1)	0(8)					
2N/O	2.50(4)	7(6)	17(3)	0.2232	2139.499	121.289	5
3N/O	2.07(1)	2(1)					
1N/O	2.44(4)	2(4)	14(2)	0.1821	1745.380	98.946	5
4N/O	2.07(1)	4(1)					
1N/O	1.54(7)	22(17)	15(2)	0.2478	2374.936	134.636	5
3N/O	2.07(1)	2(1)					
2N/O	2.47(3)	6(4)	15(2)	0.1661	1591.730	90.236	5
5N/O							
1N/O			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.07(1)	3(1)					
2N/O	2.45(3)	6(4)	13(2)	0.1664	1595.112	90.428	5
3N/O	2.08(1)	2(1)					
3N/O	2.49(3)	11(5)	16(2)	0.1664	1595.111	90.428	5
6N/O	2.04(2)	8(2)					
1N/O	2.38(2)	1(2)	9(2)	0.2667	2556.224	144.914	5
5N/O	2.06(1)	5(1)					
2N/O	2.44(3)	5(3)	12(2)	0.1951	1870.123	106.018	5
4N/O	2.07(1)	3(1)					
3N/O	2.47(3)	9(4)	14(2)	0.1584	1518.634	86.092	5

Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.16(1)	2(1)					
1S	2.02(2)	3(2)	neg10(2)	0.0878	841.931	47.729	5
2S	2.16(1)	2(1)					
2S	2.03(2)	7(2)	neg13(2)	0.0798	765.261	43.383	5
3S	2.17(1)	6(1)					
1S	1.66(8)	28(14)	neg3(3)	0.1359	1302.543	73.842	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.18(1)	6(1)					
2S	2.47(5)	18(8)	neg2(3)	0.1200	1150.615	65.229	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.18(1)	8(1)					
2S	2.48(3)	13(4)	neg3(3)	0.1232	1181.148	66.960	5
3S	2.15(1)	4(1)					
3S	2.00(2)	10(2)	neg15(2)	0.1051	1006.991	57.087	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.18(1)	10(1)					
2S	2.48(2)	10(3)	neg4(3)	0.1357	1300.960	73.752	5
4S	2.18(1)	8(1)					
3S	2.48(3)	17(5)	neg2(3)	0.1192	1142.731	64.782	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.93(3)	6(2)					5
1S	2.18(1)	0(1)	neg1(3)	0.0918	880.411	49.911	
1N/O	1.86(2)	2(1)					5
2S	2.16(1)	3(0)	neg6(2)	0.0729	698.998	39.627	
2N/O	1.87(2)	6(2)					
2S	2.17(1)	3(0)	neg6(2)	0.0819	785.397	44.525	5
3N/O	1.95(3)	1(2)					
1S	2.18(1)	0(10)	0(3)	0.0831	796.335	45.145	5

1N/O 3S	1.82(1) 2.16(1)	1(1) 5(1)	neg8(2)	0.0899	861.849	48.859	5
1N/O 4S	1.33(0.43) 2.16(2)	46(112) 8(1)	neg5(3)	0.1763	1689.856	95.799	5
4N/O 1S	1.98(4) 2.19(1)	13(3) 1(1)	1(3)	0.0851	815.436	46.227	5
2N/O 3S	2.03(0.18) 2.17(2)	32(58) 6(1)	neg3(5)	0.1385	1327.812	75.274	5
3N/O 2S	1.90(4) 2.17(1)	13(4) 3(1)	neg4(3)	0.1006	964.046	54.652	5
5N/O 1S	2.01(6) 2.19(1)	17(3) 1(1)	3(4)	0.0903	865.360	49.058	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.01(9) 2.18(2)	24(11) 4(1)	1(5)	0.1030	987.198	55.965	5
2N/O 4S	2.31(1) 2.16(2)	0(1) 11(2)	neg10(4)	0.1202	1152.462	65.334	5
3N/O 3S	2.06(0.11) 2.17(2)	33(52) 6(1)	neg2(6)	0.1359	1303.125	73.875	5
6N/O 1S	2.03(7) 2.19(1)	20(4) 1(1)	4(5)	0.0969	929.313	52.683	5
1N/O 6S	1.56(0.10) 2.15(2)	14(15) 13(1)	neg8(3)	0.2488	2385.068	135.211	5
5N/O 2S	2.06(9) 2.19(2)	25(15) 4(1)	3(7)	0.1010	968.220	54.889	5
2N/O 5S	1.54(0.27) 2.16(2)	43(51) 11(1)	neg7(4)	0.2146	2057.284	116.628	5
4N/O 3S	2.08(8) 2.18(2)	33(43) 6(1)	neg1(7)	0.1335	1279.372	72.528	5
3N/O 4S	2.31(1) 2.16(3)	2(1) 12(2)	neg13(4)	0.1212	1162.071	65.878	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.00(3)	11(3)					
1Imd	2.06(1)	1(1)	8(2)	0.2622	2192.962	124.320	5
4N/O	2.04(2)	5(3)					
1Imd	2.04(3)	0(3)					
1Imd	1.87(3)	0(2)	7(2)	0.2125	2036.823	130.235	7
3N/O	2.05(2)	3(2)					
1Imd	1.57(4)	12(7)					
1Imd	1.88(2)	0(2)					
1Imd	2.04(3)	0(3)	9(2)	0.1365	1308.647	95.944	9
2N/O	2.06(2)	1(2)					
1Imd	2.08(3)	5(3)					
1Imd	1.59(6)	12(10)					
1Imd	1.96(3)	6(3)					
1Imd	1.84(3)	3(3)	8(2)	0.1263	1210.853	104.028	11
1N/O	2.07(2)	2(2)					
1Imd	2.09(3)	6(3)					
1Imd	1.35(0.37)	47(152)					
1Imd	1.98(3)	7(4)					
1Imd	1.86(3)	4(5)					
1Imd	1.58(9)	12(22)	9(3)	0.1344	1288.745	133.692	13
4N/O	2.01(3)	9(3)					
1Imd	2.07(2)	1(1)	9(2)	0.2411	2311.512	131.041	5
3N/O	2.05(2)	3(2)					
1Imd	2.04(3)	1(2)					
1Imd	1.88(2)	0(2)	8(2)	0.1772	1698.452	108.599	7
2N/O	2.06(2)	1(2)					
1Imd	1.96(3)	7(2)					
1Imd	2.08(3)	5(2)					
1Imd	1.85(2)	4(2)	7(2)	0.1648	1580.131	115.848	9
1N/O	2.07(2)	2(2)					
1Imd	1.57(7)	16(13)					
1Imd	1.98(2)	7(2)					
1Imd	2.09(2)	6(2)					
1Imd	1.86(2)	4(3)	9(2)	0.1366	1308.959	112.457	11
0N/O							
1Imd	2.12(2)	8(2)					
1Imd	1.86(0.30)	23(113)					
1Imd	2.01(2)	9(3)					
1Imd	1.52(0.11)	13(16)					
1Imd	1.89(4)	5(3)	9(3)	0.2353	2255.521	193.779	11

3N/O	2.07(1)	1(1)					
1Imd	1.94(3)	3(4)	10(2)	0.2078	1991.574	112.903	5
2N/O	2.06(2)	0(2)					
1Imd	1.91(2)	0(2)					
1Imd	2.05(3)	1(2)	9(2)	0.1630	1562.763	99.923	7
1N/O	2.07(2)	2(2)					
1Imd	1.97(2)	8(2)					
1Imd	2.09(2)	7(2)					
1Imd	1.86(2)	5(2)	7(2)	0.1610	1542.862	113.116	9
0N/O							
1Imd	2.12(6)	8(4)					
1Imd	2.01(0.10)	8(4)					
1Imd	1.91(0.50)	3(67)					
1Imd	1.90(0.28)	4(10)	6(2)	0.2666	2555.858	187.384	9
2N/O	2.08(1)	1(1)					
1Imd	1.98(4)	3(4)	12(2)	0.2042	1957.235	110.957	5
1N/O	2.07(2)	2(2)					
1Imd	2.07(3)	2(2)					
1Imd	1.94(2)	1(2)	10(2)	0.1888	1809.426	115.695	7
0N/O							
1Imd	2.00(2)	9(2)					
1Imd	1.89(2)	6(2)					
1Imd	2.11(2)	8(2)	8(2)	0.2573	2466.834	157.730	7

Ni-N(1.8) Ni-N(1.9) Ni-S(2.0) Ni-S(2.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(2)	3(2)					
1N/O	1.96(2)	5(2)					
1S	2.02(0.22)	32(133)					
1S	2.19(2)	1(1)	neg2(9)	0.0595	570.060	41.794	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.0) Ni-S(2.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	5(1)					
1N/O	1.83(2)	3(2)					
1S	2.08(0.45)	41(281)					
1S	2.18(3)	1(1)	neg3(11)	0.066	632.542	46.375	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(2)	3(2)					
1N/O	1.96(2)	5(2)	neg3(9)	0.0576	552.607	40.515	9

1S	2.01(0.17)	30(120)					
1S	2.19(2)	1(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	2(1)					
1N/O	2.10(2)	8(2)					
1S	2.09(2)	6(1)					
1S	2.23(2)	2(2)	neg3(3)	0.0513	491.466	36.032	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	9(1)					
1S	2.10(2)	7(1)					
1S	2.24(2)	3(1)					
1C	2.94(3)	0(3)	neg2(2)	0.0349	334.763	28.761	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	8(1)					
1S	2.10(1)	6(1)					
1S	2.24(1)	3(1)					
2C	2.92(3)	5(4)	neg2(2)	0.0325	311.654	26.775	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	9(1)					
1S	2.10(2)	7(1)					
1S	2.24(2)	3(1)					
1C	2.94(3)	0(3)	neg2(2)	0.0348	333.879	28.685	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	8(1)					
1S	2.10(1)	6(1)					
1S	2.24(1)	3(1)					
2C	2.92(3)	5(4)	neg2(2)	0.0325	311.939	26.800	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-C(3.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.14(4)	7(1)					
1S	2.13(3)	5(2)	neg2(2)	0.0263	252.194	26.162	13

1S	2.22(3)	1(4)					
1C	2.83(3)	3(3)					
1C	2.97(2)	4(2)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-C(3.1)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(1)					
1S	2.12(3)	5(2)					
1S	2.22(3)	0(4)					
2C	2.84(3)	2(4)					
1C	2.96(2)	3(2)	neg3(2)	0.0242	232.351	24.104	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	8(1)					
1S	2.10(1)	6(1)					
1S	2.23(1)	3(1)					
2C	2.92(3)	5(4)					
1Cl	3.98(5)	8(5)	neg3(2)	0.0227	217.690	22.583	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	8(1)					
1S	2.10(1)	6(1)					
1S	2.24(1)	3(1)					
2C	2.93(3)	4(3)					
1Cl	3.58(3)	4(2)	neg1(2)	0.0235	225.235	23.365	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	8(1)					
1S	2.10(1)	6(1)					
1S	2.24(1)	3(1)					
2C	2.93(3)	4(3)					
1Cl	3.58(2)	4(2)	neg1(2)	0.0235	224.951	23.336	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	8(1)					
1S	2.10(1)	6(1)					
1S	2.23(1)	3(1)					
2C	2.92(3)	5(4)					
1Cl	3.98(5)	8(5)	neg2(2)	0.0227	217.889	22.603	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.10(2)	8(1)					
1S	2.10(1)	6(1)					
1S	2.23(1)	3(1)					
2C	2.92(3)	5(4)					
1Cl	3.98(5)	7(5)	neg2(2)	0.0229	219.327	22.753	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	2(1)					
1N/O	2.13(4)	7(2)					
1S	2.12(3)	4(2)					
1S	2.23(3)	0(4)					
1C	2.88(4)	1(5)					
0.25Imd	1.98(2)	4(2)	neg2(2)	0.0293	281.270	29.178	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(3)	4(2)					
1S	2.23(3)	0(3)					
2C	2.88(4)	5(5)					
0.25Imd	1.98(2)	4(2)	neg2(2)	0.0264	253.002	26.246	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(2)	5(2)					
1S	2.23(2)	0(3)					
3C	2.89(4)	9(5)					
0.25Imd	1.98(3)	4(2)	neg2(2)	0.0273	262.037	27.183	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(2)	4(2)					
1S	2.23(2)	0(3)					
2C	2.88(4)	6(5)					
0.4Imd	1.98(2)	2(2)	neg1(2)	0.0276	264.718	27.461	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(2)	4(2)					
1S	2.24(2)	0(3)					
2C	2.88(4)	6(6)					
0.5Imd	1.98(3)	1(2)	neg1(2)	0.0286	274.043	28.429	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	2(1)					
1N/O	2.13(4)	7(2)					
1S	2.12(3)	4(2)					
1S	2.23(3)	0(4)					
1C	2.88(4)	1(5)					
0.25Imd	1.98(2)	4(2)	neg2(2)	0.0293	281.012	29.152	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(3)	4(2)					
1S	2.23(3)	0(3)					
2C	2.89(4)	5(5)					
0.25Imd	1.98(2)	4(2)	neg2(2)	0.0265	254.373	26.388	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(3)	5(2)					
1S	2.23(3)	5(2)					
3C	2.89(4)	9(5)					
0.25Imd	1.98(3)	4(2)	neg2(2)	0.0277	265.613	27.554	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(2)	4(2)					
1S	2.23(2)	0(3)					
2C	2.88(4)	6(5)					
0.4Imd	1.98(3)	2(2)	neg1(2)	0.0278	266.817	27.679	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)	neg1(2)	0.0288	276.444	28.678	13

1N/O	2.13(3)	7(2)					
1S	2.12(2)	4(2)					
1S	2.24(2)	0(3)					
2C	2.88(4)	6(6)					
0.5Imd	1.98(3)	1(2)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	3(2)					
1N/O	2.09(2)	8(2)					
1S	2.09(2)	6(1)					
1S	2.23(2)	3(2)					
2C	2.92(4)	5(5)					
1Imd	1.79(0.15)	23(26)	neg4(3)	0.0314	300.905	31.215	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.35(1)	1(1)					
2S	2.18(1)	6(1)					
2C	2.86(1)	0(1)					
1Cl	3.91(1)	1(1)					
0.5Imd	1.99(1)	4(1)	neg4(1)	0.0126	120.314	12.481	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.34(1)	1(1)					
2S	2.18(1)	6(1)					
2C	2.86(1)	0(1)					
1Cl	3.90(1)	1(1)					
0.5Imd	1.99(1)	4(1)	neg5(1)	0.0123	118.024	12.244	13

Ni-N(1.8) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.89(2)	4(3)					
1S	2.07(4)	12(12)					
1S	2.20(1)	0(1)					
2C	2.88(2)	0(2)					
1Cl	3.92(2)	1(2)					
0.5Imd	2.00(1)	5(1)	neg3(2)	0.0252	241.110	25.012	13

Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(2)	4(3)					
1S	2.06(4)	13(14)					
1S	2.20(1)	0(1)					
2C	2.88(2)	0(2)	neg3(2)	0.0272	260.488	27.023	13

1Cl	3.91(2)	1(2)					
0.5Imd	2.00(1)	5(1)					

Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(2)	4(3)					
1S	2.06(4)	13(14)					
1S	2.20(1)	0(1)					
2C	2.88(2)	0(2)					
1Cl	3.91(2)	1(2)					
0.5Imd	2.00(1)	5(1)	neg3(2)	0.0272	260.488	27.023	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(2)	5(2)					
1S	2.24(2)	0(3)					
2C	2.90(4)	6(5)					
1Cl	3.58(3)	5(3)					
0.25Imd	1.98(3)	3(2)	neg1(2)	0.0228	218.723	28.630	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(3)	4(2)					
1S	2.23(3)	1(4)					
2C	2.88(4)	5(6)					
1Cl	3.48(0.14)	21(25)					
0.4Imd	1.98(3)	2(2)	neg1(2)	0.0264	252.977	33.114	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(2)	5(2)					
1S	2.24(2)	0(3)					
2C	2.90(4)	6(5)					
1Cl	3.58(3)	5(3)					
0.25Imd	1.98(3)	3(2)	neg1(2)	0.0228	218.843	28.646	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.12(3)	7(1)					
1S	2.12(2)	5(2)					
1S	2.24(2)	1(3)	neg1(2)	0.0258	247.266	32.366	15

2C	2.89(5)	7(8)					
1Cl	3.58(3)	5(3)					
0.4Imd	1.97(4)	1(3)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(3)	4(2)					
1S	2.23(3)	1(4)					
2C	2.88(4)	5(6)					
1Cl	3.45(0.18)	24(32)					
0.5Imd	1.98(3)	2(3)	neg1(2)	0.0279	267.907	35.068	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.13(3)	7(2)					
1S	2.12(3)	4(2)					
1S	2.23(3)	1(4)					
2C	2.88(4)	5(6)					
1Cl	3.45(0.17)	24(32)					
0.5Imd	1.98(3)	2(3)	neg1(2)	0.0279	267.588	35.026	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	1(1)					
1N/O	2.19(4)	5(2)					
1S	2.12(4)	2(5)					
1S	2.19(3)	3(3)					
1C	2.85(2)	3(1)					
1Cl	3.90(2)	1(1)					
0.4Imd	1.98(1)	5(1)	neg5(2)	0.009	86.600	11.336	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.18(3)	6(2)					
1S	2.13(5)	5(5)					
1S	2.18(2)	3(2)					
1C	2.85(2)	3(1)					
1Cl	3.90(1)	1(1)					
0.5Imd	1.98(1)	5(1)	neg4(2)	0.0084	80.970	10.599	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.18(1)	7(1)	neg3(1)	0.0068	65.244	8.540	15

1S	2.15(4)	13(5)					
1S	2.18(1)	4(1)					
1C	2.83(1)	4(1)					
1Cl	3.89(1)	1(1)					
1Imd	1.97(1)	2(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	2(1)					
1N/O	2.19(4)	5(2)					
1S	2.12(4)	2(5)					
1S	2.19(3)	3(3)					
1C	2.85(2)	3(1)					
1Cl	3.90(2)	1(1)					
0.4Imd	1.98(1)	5(1)	neg5(2)	0.0087	83.538	10.935	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.18(2)	6(2)					
1S	2.13(5)	5(5)					
1S	2.18(2)	3(2)					
1C	2.85(2)	3(1)					
1Cl	3.90(1)	1(1)					
0.5Imd	1.98(1)	5(1)	neg4(2)	0.0081	77.920	10.199	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.18(1)	7(1)					
1S	2.15(4)	13(5)					
1S	2.18(1)	4(1)					
1C	2.83(1)	4(1)					
1Cl	3.89(1)	1(1)					
1Imd	1.97(1)	3(1)	neg3(1)	0.0066	63.256	8.280	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.17(7)	4(3)					
1S	2.11(3)	1(4)					
1S	2.20(4)	3(4)					
2C	2.87(2)	2(2)					
1Cl	3.91(2)	2(1)					
0.25Imd	1.99(1)	6(1)	neg5(2)	0.0094	89.927	11.771	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	5(1)					
1S	2.16(5)	4(4)					
1S	2.16(2)	2(2)					
2C	2.86(2)	2(2)					
1Cl	3.91(1)	2(1)					
0.4Imd	1.99(1)	5(1)	neg3(2)	0.0085	81.868	10.716	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	6(1)					
1S	2.16(5)	5(4)					
1S	2.16(2)	3(2)					
2C	2.86(2)	1(1)					
1Cl	3.91(1)	2(1)					
0.5Imd	1.99(1)	4(1)	neg3(1)	0.0081	77.851	10.190	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.17(1)	6(1)					
1S	2.15(4)	11(5)					
1S	2.17(1)	4(1)					
2C	2.84(1)	0(1)					
1Cl	3.90(1)	1(1)					
1Imd	1.98(1)	2(1)	neg3(1)	0.0082	78.629	10.292	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.17(6)	4(3)					
1S	2.11(3)	1(4)					
1S	2.20(4)	2(4)					
2C	2.87(2)	2(2)					
1Cl	3.91(2)	2(1)					
0.25Imd	1.99(1)	6(1)	neg4(2)	0.0094	90.353	11.827	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	5(1)					
1S	2.16(5)	4(4)					
1S	2.16(2)	2(2)					
2C	2.86(2)	1(2)					
1Cl	3.91(1)	1(1)					
0.4Imd	1.99(1)	5(1)	neg3(2)	0.0085	81.949	10.727	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	6(1)					
1S	2.16(5)	5(4)					
1S	2.16(2)	3(2)					
2C	2.86(2)	1(1)					
1Cl	3.91(1)	1(1)					
0.5Imd	1.99(1)	4(1)	neg3(1)	0.0081	77.903	10.197	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.17(1)	6(1)					
1S	2.15(4)	11(5)					
1S	2.17(1)	4(1)					
2C	2.84(1)	0(1)					
1Cl	3.90(1)	0(1)					
1Imd	1.98(1)	2(1)	neg3(1)	0.0082	78.840	10.320	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	6(1)					
1S	2.16(4)	5(4)					
1S	2.17(2)	3(2)					
2C	2.86(2)	1(1)					
1Cl	3.91(1)	2(1)					
0.5Imd	1.99(1)	4(1)	neg3(1)	0.008	76.379	9.998	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	6(1)					
1S	2.16(4)	6(4)					
1S	2.17(2)	3(2)					
2C	2.86(2)	1(1)					
1Cl	3.91(1)	1(1)					
0.5Imd	1.99(1)	4(1)	neg3(1)	0.008	76.493	10.013	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.18(2)	6(2)					
1S	2.13(5)	5(5)					
1S	2.18(2)	3(2)					
1C	2.85(2)	3(1)					
1Cl	3.90(1)	1(1)	neg4(2)	0.0081	77.920	10.199	15

0.5Imd	1.98(1)	5(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.18(3)	6(2)					
1S	2.13(5)	5(5)					
1S	2.18(2)	3(2)					
1C	2.85(2)	3(1)					
1Cl	3.90(1)	1(1)					
0.5Imd	1.98(1)	5(1)	neg4(2)	0.0084	80.970	10.599	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	6(1)					
1S	2.16(5)	5(4)					
1S	2.16(2)	3(2)					
2C	2.86(2)	1(1)					
1Cl	3.91(1)	2(1)					
0.5Imd	1.99(1)	4(1)	neg3(1)	0.0081	77.851	10.190	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	6(1)					
1S	2.16(4)	5(4)					
1S	2.17(2)	3(2)					
2C	2.86(2)	1(1)					
1Cl	3.91(1)	2(1)					
0.5Imd	1.99(1)	4(1)	neg3(1)	0.008	76.379	9.998	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.17(1)	6(1)					
1S	2.15(4)	11(5)					
1S	2.17(1)	4(1)					
2C	2.84(1)	0(1)					
1Cl	3.90(1)	1(1)					
1Imd	1.98(1)	2(1)	neg3(1)	0.0082	78.684	10.299	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	2(1)					
1N/O	2.16(2)	5(1)					
1S	2.16(5)	4(4)					
1S	2.16(2)	2(2)	neg4(2)	0.0084	80.079	10.482	15

2C	2.86(2)	2(2)
1Cl	3.91(1)	2(1)
0.4Imd	1.99(1)	5(1)

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.19(7)	4(4)					
1S	2.11(1)	1(3)					
1S	2.21(3)	3(3)					
1C	2.86(2)	2(2)					
2Cl	3.92(2)	6(2)					
0.4Imd	1.99(1)	4(1)	neg5(2)	0.0104	99.603	13.038	15

Table H.3. Additional Fits for Oxidized WT NiSOD in Buffer with 50 mM Tris, 100 mM NaCl and 10 % Glycerol at pH 8.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)	10(2)	0.1726	1037.856	52.845	3
3N/O	2.08(1)	1(1)	9(2)	0.1563	851.278	43.345	3
4N/O	2.07(1)	3(1)	8(2)	0.1919	1045.349	53.226	3
5N/O	2.07(1)	5(1)	7(2)	0.2523	1374.592	69.991	3
6N/O	2.06(2)	7(1)	5(2)	0.3196	1741.218	88.658	3
7N/O	2.06(2)	10(2)	4(2)	0.3833	2088.019	106.317	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(1)	4(1)	neg10(3)	0.1608	875.998	44.604	3
3S	2.17(1)	6(1)	neg12(3)	0.1906	1038.368	52.871	3
4S	2.17(2)	9(1)	neg13(3)	0.2349	1279.572	65.152	3
5S	2.16(2)	11(1)	neg13(4)	0.2782	1515.549	77.168	3
6S	2.16(2)	13(1)	neg14(4)	0.3172	1727.933	87.982	3
7S	2.16(3)	15(2)	neg15(4)	0.3517	1915.952	97.555	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.08(1)	3(0)					
1N/O	1.95(1)	2(1)	4(1)	0.0675	367.745	20.848	5
2N/O	2.08(1)	2(0)					
2N/O	1.96(1)	1(1)	2(1)	0.0606	330.299	18.725	5
3N/O	2.09(1)	1(1)					
1N/O	1.52(7)	26(15)	11(2)	0.1348	734.578	41.644	5

4N/O	2.08(1)	3(1)					
1N/O	0.71(7)	34(32)	10(2)	0.1776	967.443	54.845	5
3N/O	2.09(1)	1(1)					
2N/O	2.44(5)	15(9)	11(2)	0.1233	671.549	38.070	5
5N/O	2.08(1)	5(1)					
1N/O	2.35(1)	1(1)	8(2)	0.1729	942.088	53.407	5
4N/O	2.08(1)	3(1)					
2N/O	2.43(4)	11(7)	10(1)	0.1427	777.195	44.060	5
3N/O	2.09(1)	1(1)					
3N/O	2.45(5)	21(10)	12(1)	0.1217	662.927	37.582	5
6N/O	2.07(1)	8(1)					
1N/O	2.35(1)	2(1)	6(2)	0.2069	1126.984	63.889	5
5N/O	2.08(1)	5(1)					
2N/O	2.42(4)	9(6)	8(2)	0.1862	1014.250	57.498	5
4N/O	2.08(1)	3(1)					
3N/O	2.45(4)	16(7)	10(1)	0.1394	759.682	43.067	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.18(1)	3(1)					
1S	2.37(3)	5(3)	neg5(3)	0.1271	692.625	39.265	5
2S	2.18(1)	3(1)					
2S	2.37(3)	13(5)	neg5(3)	0.1256	684.243	38.790	5
3S	2.19(1)	5(1)					
1S	2.40(2)	3(2)	neg6(2)	0.1237	673.636	38.189	5
4S	2.17()	9(1)					
1S	6.37(6)	7(6)	neg13(3)	0.2311	1258.945	71.370	5
3S	2.19(1)	5(1)					
2S	2.40(2)	9(3)	neg6(2)	0.1348	734.502	41.639	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.19(1)	7(1)					
2S	2.42(2)	7(2)	neg7(1)	0.1544	841.108	47.683	5
3S	2.19(1)	5(1)					
3S	2.41(3)	14(4)	neg5(2)	0.1382	752.845	42.679	5

6S	2.16(3)	13(2)					
1S	3.48(0.10)	7(10)	neg14(4)	0.3033	1652.078	93.657	5
5S	2.19(1)	9(1)					
2S	2.43(2)	7(2)	neg7(2)	0.1787	973.435	55.184	5
4S	2.19(1)	7(1)					
3S	2.43(2)	12(3)	neg6(2)	0.1607	875.460	49.630	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.92(2)	6(2)					5
1S	2.17(1)	0(0)	neg11(3)	0.0869	473.353	26.835	
1N/O	1.85(1)	1(1)					5
2S	2.16(1)	3(0)	neg14(2)	0.0938	511.100	28.974	
2N/O	1.86(2)	6(2)					
2S	2.16(1)	3(1)	neg14(3)	0.1212	660.033	37.418	5
3N/O	1.93(3)	10(3)					
1S	2.18(1)	0(0)	neg9(3)	0.0888	483.934	27.434	5
1N/O	1.83(2)	1(1)					
3S	2.16(1)	6(1)	neg15(2)	0.1406	766.175	43.435	5
1N/O	3.22(3)	2(2)					
4S	2.16(2)	9(1)	neg13(3)	0.2101	1144.588	64.887	5
4N/O	1.96(5)	15(3)					
1S	2.18(1)	0(0)	neg7(4)	0.0919	500.759	28.388	5
2N/O	4.77(4)	5(4)					
3S	2.17(1)	6(1)	neg12(3)	0.1845	1005.267	56.989	5
3N/O	1.88(6)	16(7)					
2S	2.17(1)	3(1)	neg12(4)	0.1384	754.245	42.759	5
5N/O	2.00(8)	19(4)					
1S	2.18(1)	1(0)	neg5(6)	0.0930	506.915	28.737	5
1N/O	0.68(3)	3(4)					
5S	2.16(2)	11(1)	neg14(4)	0.2701	1471.191	83.403	5
4N/O	1.93(0.14)	30(13)					
2S	2.17(2)	4(1)	neg10(5)	0.1406	766.126	43.432	5
2N/O			No Fit	No Fit	No Fit	No Fit	5

4S							
3N/O	1.12(0.30)	61(83)					
3S	2.17(2)	6(1)	neg12(3)	0.1888	1028.617	58.313	5
6N/O	2.13(2)	14(3)					
1S	2.20(1)	1(0)	6(2)	0.0901	490.944	27.832	5
1N/O	1.64(0.10)	13(14)					
6S	2.16(3)	13(2)	neg15(4)	0.3001	1634.610	92.667	5
5N/O	1.95(0.16)	35(14)					
2S	2.17(2)	4(1)	neg10(5)	0.1408	766.846	43.473	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.83(0.32)	53(67)					
3S	2.17(2)	6(1)	neg12(5)	0.1884	1026.571	58.197	5
3N/O	3.25(5)	5(5)					
4S	2.17(2)	9(1)	neg13(3)	0.2073	1129.390	64.026	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.03(3)	13(3)					
1Imd	2.07(1)	2(1)	4(2)	0.1635	983.022	55.728	5
4N/O	2.04(3)	11(3)					
1Imd	1.58(5)	15(8)					
1Imd	2.08(1)	2(1)	7(2)	0.1232	671.301	42.923	7
3N/O	2.07(1)	3(1)					
1Imd	2.05(2)	1(1)					
1Imd	1.89(2)	0(1)					
1Imd	1.63(5)	15(8)	5(2)	0.0718	391.198	28.681	9
2N/O	2.08(1)	0(1)					
1Imd	2.07(3)	1(2)					
1Imd	1.92(3)	1(2)					
1Imd	2.27(0.12)	16(25)					
1Imd	1.61(4)	14(7)	8(3)	0.0611	333.051	28.614	11
1N/O	2.09(1)	2(1)					
1Imd	2.43(6)	3(6)					
1Imd	1.98(2)	2(3)					
1Imd	2.10(3)	4(3)					
1Imd	2.24(5)	2(4)					
1Imd	1.61(4)	15(7)	12(0)	0.0670	365.038	37.868	13

4N/O	2.03(2)	10(2)					
1Imd	2.08(1)	2(1)	5(2)	0.1461	795.732	45.110	5
3N/O	2.07(1)	3(1)					
1Imd	1.89(2)	0(1)					
1Imd	2.05(2)	1(1)	3(1)	0.0917	499.339	31.928	7
2N/O	2.07(1)	0(1)					
1Imd	2.06(2)	1(1)					
1Imd	2.44(0.13)	17(22)					
1Imd	1.92(2)	0(1)	4(2)	0.0740	403.267	29.566	9
1N/O	2.08(1)	3(1)					
1Imd	2.06(5)	1(4)					
1Imd	1.94(4)	0(4)					
1Imd	2.15(0.12)	7(18)					
1Imd	1.59(5)	17(10)	7(3)	0.0778	423.596	36.392	11
0N/O							
1Imd	2.15(4)	4(4)					
1Imd	1.42(0.10)	20(17)					
1Imd	2.04(3)	6(3)					
1Imd	1.07(3)	3(3)					
1Imd	1.92(4)	3(3)	2(2)	0.1567	853.396	73.318	11
3N/O	2.04(2)	7(2)					
1Imd	2.08(1)	1(1)	6(2)	0.1390	757.489	42.942	5
2N/O	2.07(1)	0(1)					
1Imd	1.91(1)	0(1)					
1Imd	2.05(2)	1(1)	4(1)	0.0770	419.423	26.818	7
1N/O	2.08(1)	2(1)					
1Imd	2.01(4)	3(7)					
1Imd	2.11(4)	1(8)					
1Imd	1.90(3)	1(4)	3(2)	0.0884	481.387	35.293	9
0N/O							
1Imd	1.92(3)	4(2)					
1Imd	2.02(2)	8(2)					
1Imd	2.13(2)	7(2)					
1Imd	2.80(0.10)	5(11)	3(2)	0.2001	1090.181	79.927	9
2N/O	2.09(1)	1(1)					
1Imd	2.00(3)	3(3)	7(2)	0.1119	609.359	34.545	5
1N/O	2.08(1)	3(1)					
1Imd	2.07(2)	1(2)					
1Imd	1.95(2)	0(2)	4(2)	0.0936	509.678	32.589	7

0N/O							
1Imd	2.13(2)	6(2)					
1Imd	1.91(2)	4(2)					
1Imd	2.02(2)	7(2)	3(2)	0.2088	1137.300	72.719	7

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.91(3)	1(2)					
1N/O	1.86(0.36)	26(56)					
1S	2.29(5)	5(4)					
1S	2.17(2)	1(1)	neg7(6)	0.0605	329.807	24.180	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(3)	1(2)					
1N/O	1.80(0.21)	26(51)					
1S	2.17(2)	1(1)					
1S	2.29(6)	7(4)	neg8(5)	0.0602	328.058	24.052	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	2(1)					
1N/O	2.07(1)	4(1)					
1S	2.24(4)	6(3)					
1S	2.54(9)	19(14)	neg3(3)	0.0583	317.399	23.270	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(3)	1(2)					
1N/O	1.80(0.22)	26(50)					
1S	2.17(2)	1(1)					
1S	2.29(6)	7(4)	neg8(5)	0.0604	329.181	24.134	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(6)	5(60)					
1N/O	1.90(0.11)	1(7)					
1S	2.31(5)	5(4)					
1S	2.18(1)	1(3)					
1C	2.90(9)	7(12)	neg4(4)	0.0482	289.877	24.904	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(2)	0(2)					
1N/O	2.08(8)	0(20)					
1S	2.17(3)	0(6)	neg3(3)	0.0404	219.963	18.898	11

1S	2.31(4)	7(7)
2C	2.93(6)	10(8)

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(8)	5(38)					
1N/O	1.91(5)	1(6)					
1S	2.31(3)	5(4)					
1S	2.18(2)	1(3)					
3C	2.92(6)	13(7)	neg4(3)	0.0364	198.203	17.028	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(3)	3(31)					
1N/O	1.91(3)	0(4)					
1S	2.31(3)	5(4)					
1S	2.17(2)	1(3)					
4C	2.92(5)	16(7)	-4(3)	0.0341	186.019	15.981	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(0.42)	35(83)					
1N/O	1.91(3)	1(2)					
1S	2.29(4)	5(3)					
1S	2.17(2)	1(1)					
1C	2.84(7)	5(7)	neg7(4)	0.048	261.482	22.465	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(9)	6(46)					
1N/O	1.91(7)	1(6)					
1S	2.31(4)	5(4)					
1S	2.18(1)	1(2)					
2C	2.92(7)	11(8)	neg4(3)	0.0404	219.825	18.886	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(8)	5(39)					
1N/O	1.91(5)	1(6)					
1S	2.31(3)	5(4)					
1S	2.17(2)	1(2)					
3C	2.92(6)	13(7)	neg4(3)	0.0361	196.487	16.881	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.10(0)	3(0)	15(0)	0.0396	215.753	18.536	11

1N/O	1.37(3)	21(8)					
1S	1.83(1)	9(1)					
1S	2.22(4)	19(7)					
4C	3.62(5)	17(11)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(2)	1(2)					
1N/O	1.78(0.19)	29(50)					
1S	2.17(1)	1(1)					
1S	2.29(4)	7(4)					
1C	2.84(6)	5(7)	neg7(4)	0.0477	259.810	22.321	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.91(2)	1(2)					
1N/O	1.80(0.29)	39(80)					
1S	2.17(1)	1(1)					
1S	2.30(3)	6(3)					
2C	2.88(6)	10(8)	neg6(3)	0.0413	225.223	19.350	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.91(2)	1(1)					
1N/O	1.78(0.31)	44(90)					
1S	2.17(1)	1(1)					
1S	2.30(3)	6(3)					
3C	2.89(5)	13(7)	neg6(3)	0.0373	203.473	17.481	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(2)	1(4)					
1N/O	2.07(6)	3(26)					
1S	2.31(3)	5(4)					
1S	2.18(2)	0(3)					
4C	2.93(6)	15(6)	neg3(3)	0.0341	185.929	15.974	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(3)	1(6)					
1N/O	2.05(7)	3(24)					
1S	2.32(3)	6(5)					
1S	2.18(1)	0(3)					
4C	2.99(4)	9(4)					
1C	2.80(4)	1(3)	neg3(2)	0.028	152.674	15.838	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(3)	1(5)					
1N/O	2.06(6)	4(25)					
1S	2.31(3)	6(4)					
1S	2.18(1)	0(3)					
3C	2.87(4)	7(4)					
1C	3.04(3)	1(2)	neg4(2)	0.026	141.748	14.705	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(7)	3(25)					
1N/O	1.91(3)	0(4)					
1S	2.31(3)	5(3)					
1S	2.17(2)	1(3)					
4C	2.94(5)	16(6)					
1Cl	3.55(4)	8(4)	neg3(2)	0.0232	126.192	13.091	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.10(1)	4(1)					
1N/O	2.01(2)	1(2)					
1S	1.79(3)	16(3)					
1S	2.71(4)	13(5)					
4C	4.45(0.45)	42(124)					
1Cl	3.74(7)	13(10)	11(2)	0.0327	177.873	18.452	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.13(1)	7(1)					
1N/O	1.91(1)	1(1)					
1S	2.28(1)	0(1)					
1S	2.14(1)	5(1)					
4C	2.89(4)	15(5)					
1Cl	4.06(4)	7(4)	neg5(2)	0.0189	103.149	10.701	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1N/O							
1S							
1S							
4C							
1Cl			No Fit	No Fit	No Fit	No Fit	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	2(2)	neg1(2)	0.0203	122.195	12.676	13

1N/O	1.90(2)	1(1)					
1S	2.39(9)	16(10)					
1S	2.21(3)	3(2)					
1C	2.87(2)	1(2)					
0.5Imd	2.01(2)	3(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(0.10)	1(20)					
1N/O	1.90(2)	0(1)					
1S	2.32(4)	8(6)					
1S	2.18(4)	0(5)					
2C	2.88(3)	4(3)					
0.5Imd	2.01(2)	2(1)	neg3(2)	0.019	103.270	10.713	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(0.13)	0(16)					
1N/O	1.90(2)	0(1)					
1S	2.30(3)	7(4)					
1S	2.17(6)	0(3)					
3C	2.89(3)	8(3)					
0.5Imd	2.02(2)	1(2)	neg3(2)	0.018	97.970	10.163	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(1)	7(1)					
1N/O	1.90(1)	0(1)					
1S	2.30((1)	1(1)					
1S	2.16(1)	5(1)					
4C	2.88(3)	13(4)					
0.5Imd	1.99(2)	1(1)	neg4(1)	0.012	65.332	6.777	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90((1)	1(1)					
1N/O	2.16(2)	5(2)					
1S	2.31(2)	3(2)					
1S	2.16(1)	4(1)					
4C	2.90(3)	13(4)					
1Imd	2.01(2)	2(2)	neg3(1)	0.0156	84.792	8.796	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(2)	1(1)					
1N/O	2.07(2)	2(2)					
1S	2.38(9)	17(10)					
1S	2.20(3)	3(2)	neg1(2)	0.0211	114.718	11.901	13

1C	2.88(2)	1(2)					
0.5Imd	2.01(2)	3(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(2)	0(1)					
1N/O	2.11(0.14)	2(33)					
1S	2.31(4)	8(4)					
1S	2.18(7)	0(4)					
2C	2.89(3)	4(3)					
0.5Imd	2.02(2)	2(1)	neg3(2)	0.019	103.671	10.755	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(1)	1(1)					
1N/O	2.17(1)	6(1)					
1S	2.31(2)	3(2)					
1S	2.17(1)	4(1)					
3C	2.90(3)	10(4)					
0.5Imd	2.01(1)	2(1)	neg3(1)	0.0142	77.278	8.017	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(1)	7(1)					
1N/O	1.90(1)	0(1)					
1S	2.30(1)	1(1)					
1S	2.16(1)	5(1)					
4C	2.88(3)	13(4)					
0.5Imd	1.99(2)	1(1)	neg4(1)	0.012	65.230	6.767	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(1)	0(1)					
1N/O	2.16(2)	5(2)					
1S	2.31(2)	4(2)					
1S	2.17(1)	3(1)					
4C	2.89(3)	9(4)					
1Imd	2.01(2)	2(2)	neg2(1)	0.0156	84.767	8.794	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(1)	1(1)					
1N/O	2.17(2)	6(2)					
1S	2.16(2)	4(2)					
1S	2.30(2)	5(3)					
4C	2.90(3)	14(4)					
1Imd	2.02(1)	2(1)	neg3(1)	0.0174	94.666	9.820	13

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.92(3)	1(4)					
1N/O	2.08(2)	3(1)					
1S	2.15(0.10)	6(9)					
1S	2.26(9)	14(28)					
4C	2.90(4)	13(5)					
1Imd	2.02(2)	1(1)	neg4(2)	0.0214	116.370	12.072	13

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.15(1)	6(1)					
1N/O	1.89(1)	0(1)					
1S	2.151)	4(1)					
1S	2.30(1)	3(2)					
4C	2.88(3)	12(3)					
1Imd	1.99(2)	1(2)	neg5(1)	0.0133	72.278	7.498	13

Ni-N(1.9) Ni-N(2.1) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.64(0.11)	28(20)					
1N/O	1.89(1)	0(1)					
1S	2.18(1)	0(1)					
1S	2.31(2)	7(3)					
4C	2.88(3)	10(3)					
1Imd	2.01(2)	1(1)	neg5(1)	0.0209	113.630	11.788	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(7)	5(31)					
1N/O	1.91(3)	0(4)					
1S	2.31(3)	5(3)					
1S	2.17(2)	1(2)					
4C	2.93(5)	16(6)					
1Cl	3.55(4)	8(4)					
1Cl	4.08(5)	8(6)	neg4(2)	0.0182	98.927	12.949	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.91(2)	1(1)					
1N/O	1.85(0.66)	57(159)					
1S	2.17(1)	1(1)					
1S	2.30(3)	6(3)					
3C	2.90(5)	13(7)					
1Cl	3.54(5)	8(5)					
1Cl	4.06(5)	7(6)	neg5(3)	0.0229	124.946	16.355	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(2)	1(4)					
1N/O	2.06(6)	3(22)					
1S	2.32(3)	5(3)					
1S	2.18(1)	0(2)					
4C	2.94(5)	16(6)					
1Cl	3.55(4)	8(4)					
1Cl	4.08(5)	8(6)	neg3(2)	0.0177	96.283	12.603	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(1)	7(1)					
1N/O	1.90(1)	0(1)					
1S	2.30(1)	1(1)					
1S	2.16(1)	5(1)					
4C	2.89(2)	13(3)					
1Cl	3.53(3)	10(4)					
0.5Imd	2.00(2)	1(1)	neg4(1)	0.0086	46.680	6.110	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(1)	1(1)					
1N/O	2.16(1)	6(1)					
1S	2.30(1)	3(2)					
1S	2.16(1)	4(1)					
4C	2.91(2)	14(4)					
1Cl	3.53(3)	10(4)					
0.5Imd	2.01(1)	1(1)	neg3(1)	0.0086	46.955	6.146	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.16(1)	7(1)					
1N/O	1.90(1)	0(1)					
1S	2.30(1)	1(1)					
1S	2.16(1)	5(1)					
4C	2.89(2)	13(3)					
1Cl	3.53(3)	10(4)					
0.5Imd	2.00(2)	1(1)	neg4(1)	0.0085	46.532	6.091	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(1)	1(1)					
1N/O	2.16(1)	6(1)					
1S	2.30(1)	3(2)					
1S	2.16(1)	4(1)					
4C	2.91(2)	14(4)					
1Cl	3.53(3)	10(4)					
0.5Imd	2.01(1)	1(1)	neg3(1)	0.0086	46.863	6.134	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.91(2)	1(1)					
1N/O	1.90(0.53)	43(84)					
1S	2.31(3)	5(4)					
1S	2.17(1)	1(1)					
4C	2.89(5)	16(7)					
1Cl	4.04(7)	9(7)					
0.5Imd	2.43(9)	4(8)	neg6(3)	0.024	130.726	17.111	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.91(4)	4(3)					
1N/O	1.66(7)	21(13)					
1S	2.31(2)	4(2)					
1S	2.18(1)	1(0)					
3C	2.84(3)	7(3)					
1C	3.04(3)	0(2)					
1Imd	1.95(5)	5(6)	neg5(1)	0.0165	89.765	11.750	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(2)	1(1)					
1N/O	1.52(0.85)	79(171)					
1S	2.33(2)	5(2)					
1S	2.19(1)	1(1)					
3C	2.88(3)	5(3)					
1C	3.10(6)	1(5)					
0.5Imd	2.00(3)	2(2)	neg4(2)	0.0171	93.329	12.216	15

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.94(2)	5(2)					
1S	2.34(3)	4(3)					
1S	2.19(1)	1(1)					
3C	2.90(5)	13(7)					
1Cl	3.53(7)	12(11)					
1Cl	4.11(0.24)	20(36)					
1Imd	2.42(8)	6(10)	neg5(2)	0.0225	122.637	16.053	15

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(2)	5(1)					
1S	2.20(1)	1(0)					
1S	2.43(3)	6(3)					
4C	2.96(4)	16(6)					
1Cl	3.47(2)	1(2)	neg3(1)	0.0156	84.782	11.098	15

1Cl	3.67(5)	8(7)					
1Imd	2.49(2)	2(1)					

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(2)	5(1)					
1S	2.20(1)	1(0)					
1S	2.43(3)	6(3)					
4C	2.96(4)	17(6)					
1Cl	3.47(2)	1(2)					
1Cl	3.67(5)	8(7)					
1Imd	2.49(2)	2(1)	neg3(1)	0.0155	84.632	11.078	15

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.91(2)	6(2)					
1S	2.19(1)	1(1)					
1S	2.36(4)	9(5)					
4C	2.91(4)	10(5)					
1Cl	3.54(4)	3(3)					
1Cl	3.35(6)	7(6)					
1Imd	2.05(3)	1(3)	neg3(2)	0.0394	214.412	28.066	15

Ni-N(1.9) Ni-S(2.2) Ni-S(2.3) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.94(2)	5(1)					
1S	2.19(1)	1(0)					
1S	2.42(3)	10(5)					
4C	2.87(9)	24(13)					
1Cl	3.47(2)	3(2)					
1Cl	3.15(6)	14(8)					
1Imd	2.49(2)	1(1)	neg5(2)	0.0152	82.774	10.834	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.50(4)	0(4)					
1N/O	2.29(4)	2(3)					
2S	2.19(2)	3(2)					
4C	2.77(3)	8(3)					
1Cl	3.13(4)	7(4)					
1Cl	3.96(0.17)	20(30)					
1Imd	1.90(3)	4(3)	neg9(2)	0.024	130.930	17.138	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(2)	3(2)					
1N/O	1.64(4)	12(5)					
2S	2.21(1)	2(1)	neg2(2)	0.0155	84.649	11.080	15

4C	1.27(9)	114(41)					
1Cl	2.38(1)	1(1)					
1Cl	2.57(2)	5(2)					
1Imd	2.00(2)	3(2)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(2)	1(4)					
1N/O	2.06(5)	4(20)					
1S	2.31(2)	6(2)					
1S	2.18(1)	0(2)					
3C	2.88(3)	7(3)					
1C	3.04(2)	1(2)					
1Cl	3.54(3)	8(3)					
1Cl	4.08(4)	8(5)	neg4(2)	0.0101	54.996	9.752	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(2)	1(2)					
1N/O	2.44(2.3)	64(605)					
1S	2.32(2)	5(3)					
1S	2.18(1)	0(1)					
3C	2.87(5)	6(4)					
1C	3.06(0.13)	5(14)					
1Cl	4.00(9)	13(14)					
0.5 Imd	2.01(4)	1(2)	neg4(5)	0.0136	74.027	13.126	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(1)	0(1)					
1N/O	2.18(2)	6(2)					
1S	2.17(2)	4(1)					
1S	2.31(2)	5(3)					
3C	2.87(3)	5(2)					
1C	3.08(5)	1(5)					
1Cl	4.08(0.14)	22(25)					
0.5 Imd	1.99(2)	3(2)	neg3(1)	0.0085	46.272	8.205	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.15(2)	6(1)					
1N/O	1.89(1)	0(1)					
1S	2.15(1)	4(1)					
1S	2.29(2)	3(2)					
4C	2.88(2)	12(3)					
1Cl	3.54(3)	10(4)					
1Cl	3.98(9)	17(15)					
0.5 Imd	2.00(2)	1(2)	neg5(1)	0.0077	42.106	7.466	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(3.5) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.15(2)	6(2)					
1N/O	1.89(1)	0(1)					
1S	2.16(1)	4(1)					
1S	2.30(2)	4(2)					
3C	2.87(3)	8(3)					
1Cl	3.54(4)	9(5)					
1Cl	3.96(0.10)	17(16)					
0.5 Imd	2.00(2)	1(2)	neg5(1)	0.0092	49.922	8.852	15

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.93(2)	6(2)					
1S	2.18(1)	1(1)					
1S	2.33(5)	7(4)					
3C	2.89(6)	13(8)					
1C	3.73(4)	1(3)					
1Cl	3.60(0.10)	13(20)					
1Cl	4.03(8)	7(8)					
1Imd	2.42(0.12)	9(18)	neg6(2)	0.0225	122.672	21.752	15

APPENDIX I

ADDITIONAL FIT TABLES FOR H53A NiSOD

Table I.1. Additional Fits for Reduced H53A-NiSOD in Buffer with 50 mM Tris, 100 mM NaCl and 10 % Glycerol at pH 8.0.

Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

	Ni-N(2.0)						
N	**Radius Å**	**σ^2 (x10^{-3} $Å^2$)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(1)	0(1)	20(3)	0.3393	23846.535	1214.204	3
3N/O	2.06(1)	2(1)	16(2)	0.3031	21302.646	1084.676	3
4N/O	2.05(2)	4(1)	14(2)	0.3127	21974.352	1118.877	3
5N/O	2.04(1)	6(2)	12(0)	0.3436	24144.064	1229.353	3
6N/O	2.03(2)	8(2)	10(2)	0.3866	27165.310	1383.187	3
7N/O	2.02(2)	10(2)	8(3)	0.4369	30699.021	1563.115	3

	Ni-S(2.2)						
N	**Radius Å**	**σ^2 (x10^{-3} $Å^2$)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.17(1)	3(1)	0(3)	0.1555	10930.582	556.557	3
3S	2.16(1)	6(1)	neg2(2)	0.1369	9621.539	489.904	3
4S	2.16(1)	8(1)	neg4(2)	0.1558	10946.171	557.351	3
5S	2.15(2)	10(1)	neg5(3)	0.1893	13305.885	677.501	3
6S	2.15(2)	12(1)	neg6(3)	0.2281	16027.698	816.089	3
7S	2.14(2)	14(1)	neg7(3)	0.2677	18809.552	957.734	3

	Ni-N(2.0) Ni-N(2.2)						
	r(Å)	**σ^2(x10^{-3} $Å^2$)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.07(2)	0(1)					
1N/O	2.41(3)	1(2)	18(3)	0.2829	19883.332	1127.195	5
2N/O	2.08(1)	0(1)					
2N/O	2.51(6)	9(9)	20(3)	0.2847	20005.796	1134.138	5
3N/O	2.05(1)	2(1)					
1N/O	2.39(2)	2(2)	14(2)	0.2172	15264.772	865.367	5
4N/O	2.06(2)	3(1)					
1N/O	1.54(7)	20(16)	17(2)	0.2710	19044.056	1079.617	5
3N/O	2.07(1)	2(1)					
2N/O	2.47(4)	7(6)	17(2)	0.2203	15483.350	877.758	5
5N/O	2.04(2)	6(2)					
1N/O	3.92(8)	1(7)	12(2)	0.3305	23225.062	1316.640	5

4N/O	2.06(1)	3(1)					
2N/O	2.43(3)	4(3)	14(2)	0.2023	14214.321	805.817	5
3N/O	2.07(1)	1(1)					
3N/O	2.50(4)	11(7)	18(2)	0.2170	15249.420	864.497	5
6N/O	2.02(2)	8(1)					
1N/O	2.36(1)	3(1)	9(2)	0.2175	15281.940	866.340	5
5N/O	2.04(1)	5(1)					
2N/O	2.40(2)	1(2)	12(2)	0.2025	14228.226	806.605	5
4N/O	2.06(1)	3(1)					
3N/O	2.47(3)	9(5)	16(2)	0.1956	13746.118	779.274	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.16(1)	0(0)					
1S	2.02(1)	1(1)	neg8(2)	0.0504	3540.788	200.729	5
2S	2.17(1)	1(0)					
2S	2.04(1)	4(1)	neg10(2)	0.0534	3755.937	212.926	5
3S	2.17(1)	5(1)					
1S	2.48(5)	10(6)	neg1(3)	0.1178	8276.494	469.198	5
4S	2.17(1)	8(1)					
1S	2.46(2)	5(2)	neg2(3)	0.1084	7616.342	431.774	5
3S	2.16(1)	3(1)					
2S	2.01(1)	5(1)	neg11(2)	0.0774	5436.679	308.208	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.17(1)	7(1)					
2S	2.48(3)	13(4)	neg1(3)	0.1086	7628.175	432.445	5
3S	2.16(1)	3(1)					
3S	2.02(2)	8(2)	neg12(2)	0.1075	7552.644	428.163	5
6S	2.13(1)	8(1)					
1S	1.94(2)	3(1)	neg11(2)	0.1673	11757.261	666.525	5
5S	2.17(1)	9(1)					
2S	2.47(2)	9(3)	neg3(2)	0.1132	7956.619	451.065	5
4S	2.16(2)	8(1)					
3S	1.74(8)	50(27)	neg1(4)	0.1459	10251.918	581.186	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.94(1)	2(1)					5
1S	2.19(1)	1(0)	2(2)	0.0494	3472.390	196.851	
1N/O	1.88(1)	0(1)					5
2S	2.17(1)	2(0)	neg2(1)	0.0494	3468.734	196.644	
2N/O	1.90(2)	4(1)					
2S	2.17(1)	3(0)	neg2(2)	0.0658	4622.540	262.054	5
3N/O	1.95(2)	6(1)					
1S	2.19(1)	0(0)	3(2)	0.0501	3517.572	199.413	5
1N/O	1.86(1)	0(1)					
3S	2.16(1)	5(0)	neg4(2)	0.0817	5742.546	325.548	5
1N/O	2.31(1)	3(1)					
4S	2.14(2)	10(1)	neg9(3)	0.0659	4629.318	262.438	5
4N/O	1.97(2)	9(2)					
1S	2.19(1)	0(0)	4(2)	0.0641	4501.712	255.204	5
2N/O	2.02(0.11)	23(33)					
3S	2.17(2)	6(1)	0(4)	0.1238	8703.132	493.385	5
3N/O	1.93(4)	11(3)					
2S	2.18(1)	3(1)	0(3)	0.0909	6385.808	362.014	5
5N/O	1.99(4)	13(2)					
1S	2.19(1)	0(1)	5(3)	0.0801	5628.398	319.077	5
1N/O	2.79(3)	0(3)					
5S	2.15(2)	10(1)	neg5(3)	0.1654	11623.377	658.935	5
4N/O	2.05(7)	18(10)					
2S	2.19(1)	4(1)	6(5)	0.0904	6354.390	360.233	5
2N/O	2.31(1)	1(1)					
4S	2.13(2)	11(1)	neg12(3)	0.0633	4451.377	252.351	5
3N/O	2.06(7)	24(35)					
3S	2.17(2)	6(1)	1(6)	0.1192	8373.457	474.695	5
6N/O	2.01(5)	17(3)					
1S	2.19(1)	0(1)	6(3)	0.0948	6664.894	377.836	5
1N/O	1.58(9)	13(13)	neg7(3)	0.2183	15343.136	869.810	5

6S	2.14(2)	12(1)					
5N/O	2.08(5)	20(9)					
2S	2.19(1)	3(1)	8(4)	0.0863	6062.634	343.694	5
2N/O	2.31(1)	1(1)					
5S	2.14(2)	13(1)	neg11(3)	0.0617	4332.597	245.617	5
4N/O	2.09(5)	23(31)					
3S	2.18(2)	6(1)	3(7)	0.1140	8008.927	454.030	5
3N/O	2.15(0.23)	20(44)					
4S	2.16(2)	7(1)	neg1(9)	0.1412	9920.811	562.415	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	1.99(2)	8(2)					
1Imd	2.07(2)	2(1)	9(2)	0.2593	18218.539	1032.818	5
4N/O	2.02(3)	6(4)					
1Imd	1.91(4)	0(3)					
1Imd	2.06(2)	2(1)	8(2)	0.2125	14936.045	955.012	7
3N/O	2.03(2)	4(2)					
1Imd	1.58(8)	17(13)					
1Imd	2.06(2)	2(1)					
1Imd	1.91(3)	1(2)	11(2)	0.1431	10056.349	737.288	9
2N/O	2.05(2)	1(2)					
1Imd	2.08(3)	5(3)					
1Imd	1.60(0.10)	16(15)					
1Imd	1.85(4)	3(5)					
1Imd	1.96(4)	6(5)	9(2)	0.1384	9724.035	835.423	11
1N/O	2.07(3)	2(3)					
1Imd	1.98(3)	9(4)					
1Imd	1.87(3)	6(5)					
1Imd	1.72(0.20)	10(23)					
1Imd	1.47(0.14)	13(18)					
1Imd	2.09(2)	8(3)	9(3)	0.1371	9634.677	999.484	13
4N/O	2.00(2)	6(2)					
1Imd	2.08(1)	2(1)	11(2)	0.2270	15951.994	904.326	5
3N/O	2.03(2)	3(2)					
1Imd	2.06(2)	2(1)					
1Imd	1.90(3)	1(2)	10(2)	0.1734	12186.681	779.217	7
2N/O	2.05(2)	1(2)	9(2)	0.1701	11950.908	876.189	9

1Imd	1.95(0.14)	2(11)					
1Imd	2.08(3)	3(5)					
1Imd	1.89(0.18)	2(25)					
1N/O	2.07(2)	2(2)					
1Imd	1.98(3)	8(3)					
1Imd	1.87(3)	5(3)					
1Imd	2.09(2)	7(2)					
1Imd	1.58(0.11)	21(21)	10(2)	0.1371	9635.585	827.824	11
0N/O							
1Imd	2.11(2)	9(2)					
1Imd	1.89(2)	7(3)					
1Imd	1.81(0.21)	14(50)					
1Imd	2.00(2)	10(3)					
1Imd	1.49(0.13)	12(12)	10(3)	0.2065	14511.493	1246.729	11
3N/O	2.01(2)	4(2)					
1Imd	2.08(2)	2(1)	12(2)	0.2191	15396.085	872.811	5
2N/O	2.05(2)	1(2)					
1Imd	1.92(2)	2(2)					
1Imd	2.06(2)	3(1)	11(2)	0.1508	10599.193	677.713	7
1N/O	2.06(2)	2(2)					
1Imd	1.91(0.22)	0(25)					
1Imd	1.97(0.18)	3(17)					
1Imd	2.09(5)	4(6)	10(2)	0.1633	11476.338	841.395	9
0N/O							
1Imd	2.00(3)	10(3)					
1Imd	1.88(0.14)	7(31)					
1Imd	1.90(4)	7(3)					
1Imd	2.11(2)	9(3)	8(2)	0.2357	16565.951	1214.544	9
2N/O	2.02(3)	3(3)					
1Imd	2.09(2)	2(1)	14(3)	0.2459	17277.722	979.482	5
1N/O	2.07(2)	2(2)					
1Imd	1.94(2)	3(1)					
1Imd	2.07(2)	4(1)	12(2)	0.1683	11830.079	756.416	7
0N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O	1.87(1)	3(1)	1(2)	0.0273	1917.607	164.748	11

1N/O	2.12(2)	7(2)					
1S	2.11(2)	5(1)					
1S	2.23(2)	1(2)					
1C	2.94(4)	2(4)					
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(2)	5(1)					
1S	2.22(2)	1(2)					
2C	2.94(4)	6(4)	0(2)	0.0252	1774.147	152.423	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(2)					
1S	2.11(2)	5(1)					
1S	2.23(2)	1(2)					
1C	2.94(4)	2(4)	1(2)	0.0273	1917.607	164.748	11
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(2)	5(1)					
1S	2.22(2)	1(2)					
2C	2.94(4)	6(4)	0(2)	0.0252	1774.147	152.423	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(2)					
1S	2.11(2)	5(1)					
1S	2.23(2)	1(2)					
1C	2.94(4)	2(4)	1(2)	0.0273	1921.235	165.060	11
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(2)	5(1)					
1S	2.22(2)	1(2)					
2C	2.94(4)	6(5)	0(2)	0.0256	1796.897	154.377	11

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(2)	8(2)					
1S	2.11(1)	5(1)					
1S	2.24(2)	7(1)					
1C	2.90(4)	8(5)	neg3(2)	0.0234	1644.183	141.257	11

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(2)	8(2)					
1S	2.11(1)	5(1)					
1S	2.24(2)	6(1)					
2C	2.90(4)	8(5)	neg3(2)	0.0234	1645.413	141.363	11

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(4)	5(2)					
1N/O	1.98(3)	7(2)					
1S	1.99(4)	4(9)					
1S	2.19(1)	3(1)					
2C	2.92(4)	8(6)	neg1(2)	0.0257	1807.808	155.315	11

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(2)	9(2)					
1S	2.11(1)	5(1)					
1S	2.24(2)	7(1)					
2C	2.90(4)	8(5)	neg2(2)	0.0220	1548.844	133.066	11

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(2)	9(2)					
1S	2.11(1)	5(1)					
1S	2.24(2)	7(1)					
2C	2.90(4)	8(6)	neg3(2)	0.0221	1550.779	133.232	11

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(2)	8(2)					
1S	2.11(1)	5(1)					
1S	2.24(2)	7(1)					
1C	2.89(5)	3(5)	neg3(2)	0.0255	1788.537	153.659	11
1N/O	1.85(1)	3(1)					
1N/O	2.27(2)	8(2)					
1S	2.11(1)	5(1)					
1S	2.24(2)	6(1)					
2C	2.90(4)	8(5)	neg3(2)	0.0234	1644.410	141.277	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(2)	5(1)					
1S	2.22(1)	1(2)					
2C	2.94(3)	7(4)					
1Cl	4.00(2)	4(2)	0(1)	0.0114	803.381	83.341	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(2)	5(1)					
1S	2.22(1)	1(2)					
2C	2.94(3)	7(4)					
1Cl	3.99(2)	4(2)	0(1)	0.0115	810.522	84.082	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(2)	8(2)					
1S	2.11(1)	5(1)					
1S	2.25(2)	7(1)					
2C	2.90(4)	8(5)					
1Cl	3.50(4)	9(6)	neg2(2)	0.0181	1269.982	131.746	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(1)					
1S	2.25(1)	7(1)					
2C	2.90(3)	8(3)					
1Cl	3.97(2)	4(2)	neg3(1)	0.0076	533.036	55.296	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(1)					
1S	2.25(1)	7(1)					
2C	2.90(3)	8(3)	neg3(1)	0.0077	537.862	55.797	13

1Cl	3.97(2)	3(2)					

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(1)					
1S	2.25(1)	7(1)					
2C	2.90(3)	8(3)					
1Cl	3.97(2)	4(2)	neg3(1)	0.0076	531.933	55.182	13

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.91(2)	7(3)					
1Cl	3.98(2)	4(2)	neg2(1)	0.0070	494.926	51.343	13

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.91(2)	7(3)					
1Cl	3.98(2)	3(2)	neg2(1)	0.0071	500.623	51.934	13

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(3)	5(1)					
1N/O	1.98(2)	7(1)					
1S	1.99(3)	3(6)					
1S	2.19(1)	3(1)					
2C	2.92(3)	8(4)					
1Cl	3.99(2)	4(2)	neg1(1)	0.0113	795.952	82.571	13

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.90(2)	8(3)	neg2(1)	0.0065	457.424	47.452	13

1Cl	3.98(2	4(2)					

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.90(3)	8(3)					
1Cl	3.97(2)	3(2)	neg2(1)	0.0066	462.998	48.031	13

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.90(3)	8(3)					
1Cl	3.98(2)	4(2)	neg2(1)	0.0065	456.217	47.327	13

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.90(3)	8(3)					
1Cl	3.97(2)	3(2)	neg2(1)	0.0066	461.840	47.910	13

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.98(2)	4(2)	neg2(1)	0.0065	457.424	47.452	13

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.90(3)	8(3)	neg2(1)	0.0066	462.998	48.031	13

1Cl	3.97(2)	3(2)					

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.90(3)	8(3)					
1Cl	3.97(2)	4(2)	neg3(1)	0.0063	446.109	46.279	13

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(1)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(1)					
1S	2.24(1)	7(1)					
2C	2.90(3)	8(3)					
1Cl	3.97(2)	3(2)	neg2(1)	0.0066	461.840	47.910	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	4.00(2)	5(2)					
1Cl	3.51(4)	12(6)	0(1)	0.0072	507.163	66.386	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(1)	7(1)					
1N/O	1.87(1)	3(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.92(2)	7(3)					
1Cl	3.99(2)	4(2)					
1Cl	3.50(3)	12(4)	neg1(1)	0.0045	316.213	41.391	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)	0(1)	0.0072	508.908	66.614	15

1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	3.51(4)	12(6)					
1Cl	4.00(2)	5(2)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	3.51(4)	12(6)					
1Cl	4.00(2)	4(2)	0(1)	0.0073	511.613	66.968	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	6(3)					
1Cl	3.51(4)	12(6)					
1Cl	4.00(2)	5(2)	0(1)	0.0073	511.710	66.981	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	3.51(4)	12(6)					
1Cl	4.00(2)	4(2)	0(1)	0.0073	514.379	67.330	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(1)	7(1)					
1N/O	1.87(1)	3(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.92(2)	7(3)					
1Cl	3.99(2)	5(2)					
1Cl	3.50(3)	12(4)	neg1(1)	0.0045	313.904	41.089	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	4.00(2)	4(2)					
1Cl	3.51(4)	12(6)	0(1)	0.0073	513.790	67.253	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(1)	7(1)					
1N/O	1.87(1)	3(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.92(2)	7(3)					
1Cl	3.50(3)	12(5)					
1Cl	3.99(2)	5(2)	neg1(1)	0.0045	316.150	41.383	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	3.51(4)	12(6)					
1Cl	4.00(2)	4(2)	0(1)	0.0073	515.602	67.490	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	3.51(4)	12(6)					
1Cl	4.00(2)	5(2)	0(1)	0.0073	515.831	67.520	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.87(1)	3(1)					
1N/O	2.12(2)	7(1)					
1S	2.11(1)	5(1)					
1S	2.22(1)	1(1)					
2C	2.94(3)	7(3)					
1Cl	3.51(4)	12(6)					
1Cl	4.00(2)	4(2)	0(1)	0.0074	518.494	67.869	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(1)					
1S	2.25(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.97(2)	4(1)					
1Cl	3.50(3)	11(4)	neg2(1)	0.0045	317.223	41.523	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.97(2)	3(1)					
1Cl	3.50(3)	11(4)	neg2(1)	0.0045	316.492	41.428	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	4(1)	neg2(1)	0.0046	320.159	41.908	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)	neg2(1)	0.0045	319.335	41.800	15

2C	2.90(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	3(1)					

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	4(1)	neg2(1)	0.0046	322.797	42.253	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	3(1)	neg2(1)	0.0046	321.921	42.138	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.97(2)	4(1)					
1Cl	3.50(3)	11(4)	neg2(1)	0.0045	313.548	41.042	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.97(2)	3(1)					
1Cl	3.50(3)	11(4)	neg2(1)	0.0045	312.869	40.953	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	4(1)	neg2(1)	0.0045	316.524	41.432	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	3(1)	neg2(1)	0.0045	315.752	41.331	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	4(1)	neg2(1)	0.0045	319.189	41.781	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	3(1)					
1N/O	2.27(1)	8(1)					
1S	2.11(1)	5(0)					
1S	2.25(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.97(2)	3(1)	neg2(1)	0.0045	318.364	41.673	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)	neg2(1)	0.0039	271.595	35.551	15

1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.98(2)	4(1)					
1Cl	3.50(3)	11(4)					

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.98(1)	4(1)					
1Cl	3.50(3)	11(4)	neg2(1)	0.0039	272.053	35.611	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(2)	4(1)	neg2(1)	0.0039	274.306	35.906	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(2)	4(1)	neg2(1)	0.0039	274.677	35.954	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)	neg2(1)	0.0039	277.335	36.302	15

1Cl	3.98(2)	4(1)					

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(2)	4(1)	neg2(1)	0.0040	277.657	36.344	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.98(1)	4(1)					
1Cl	3.50(3)	11(4)	neg2(1)	0.0038	266.706	34.911	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(3)	5(1)					
1N/O	1.99(2)	7(1)					
1S	1.99(3)	3(6)					
1S	2.19(1)	3(1)					
2C	2.93(3)	8(4)					
1Cl	3.99(2)	4(2)					
1Cl	3.50(4)	12(5)	neg1(1)	0.0073	516.143	67.561	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0038	269.470	35.273	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(3)	5(1)					
1N/O	1.99(2)	7(1)					
1S	1.99(3)	3(6)					
1S	2.19(1)	3(1)					
2C	2.93(3)	8(4)					
1Cl	3.50(4)	12(5)					
1Cl	3.99(2)	4(2)	neg1(1)	0.0074	518.943	67.928	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(2)	4(1)	neg2(1)	0.0039	272.530	35.673	15

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.27(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0039	272.894	35.721	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.98(1)	4(1)					
1Cl	3.50(3)	11(3)	neg2(1)	0.0035	242.858	31.789	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)	neg2(1)	0.0035	243.148	31.827	15

1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.98(1)	4(1)					
1Cl	3.50(3)	11(3)					

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0035	245.408	32.123	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(3)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0035	245.609	32.149	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0035	248.144	32.481	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0035	248.296	32.501	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.98(1)	4(1)					
1Cl	3.50(3)	11(3)	neg2(1)	0.0034	239.128	31.300	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.98(1)	4(1)					
1Cl	3.50(3)	11(3)	neg2(1)	0.0034	239.457	31.344	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(3)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0034	241.722	31.640	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(3)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0034	241.962	31.672	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(4)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0035	244.488	32.002	15

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.91(2)	8(3)					
1Cl	3.50(3)	11(3)					
1Cl	3.98(1)	4(1)	neg2(1)	0.0035	244.679	32.028	15

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(0)	5(0)					
1S	2.24(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.97(1)	4(1)					
1Cl	3.50(3)	11(3)	neg2(1)	0.0034	241.293	31.584	15

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.4) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.97(1)	4(1)					
1Cl	3.50(3)	11(3)	neg2(1)	0.0034	241.390	31.597	15

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)	neg2(1)	0.0035	243.766	31.908	15

2C	2.90(2)	8(3)					
1Cl	2.50(3)	11(3)					
1Cl	3.97(1)	4(1)					

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.50(3)	11(3)					
1Cl	3.97(1)	4(1)	neg2(1)	0.0035	243.774	31.909	15

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(3.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	2(0)					
1N/O	2.26(1)	9(5)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.50(3)	11(3)					
1Cl	3.97(1)	4(1)	neg2(1)	0.0035	246.264	32.235	15

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Cl(4.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	3(0)					
1N/O	2.26(1)	9(1)					
1S	2.11(1)	5(0)					
1S	2.24(1)	7(1)					
2C	2.90(2)	8(3)					
1Cl	3.50(3)	11(3)					
1Cl	3.97(1)	4(1)	neg2(1)	0.0035	246.223	32.230	15

Table I.2. Additional Fits for As Isolated H53A-NiSOD in Buffer with 50 mM Tris, 100 mM NaCl and 10 % Glycerol at pH 8.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(2)	2(1)	8(3)	0.2920	1076.033	54.789	3
3N/O	2.05(1)	4(1)	8(2)	0.2416	1041.026	53.006	3
4N/O	2.05(2)	6(1)	7(2)	0.2525	1088.408	55.419	3
5N/O	2.04(2)	9(2)	6(2)	0.2941	1267.426	64.534	3

6N/O	2.04(2)	11(2)	5(2)	0.3472	1496.401	76.193	3
7N/O	2.03(3)	14(2)	4(3)	0.4016	1730.722	88.124	3

Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.16(2)	6(1)	neg10(4)	0.2463	1061.560	54.052	3
3S	2.16(2)	9(1)	neg10(3)	0.2157	929.808	47.343	3
4S	2.16(2)	12(1)	neg11(3)	0.2245	967.331	49.254	3
5S	2.16(2)	14(1)	neg11(3)	0.2488	1072.126	54.590	3
6S	2.16(3)	16(2)	neg12(4)	0.2786	1200.517	61.127	3
7S	2.16(3)	18(2)	neg13(4)	0.3093	1333.059	67.876	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.06(0.13)	3(6)					
1N/O	2.00(0.26)	5(31)	6(3)	0.2416	1041.178	59.025	5
2N/O	2.05(3)	3(2)					
2N/O	1.98(6)	10(10)	4(3)	0.2381	1025.983	58.163	5
3N/O	2.06(1)	4(1)					
1N/O	2.48(2)	0(2)	9(2)	0.1445	622.889	35.312	5
4N/O	2.06(1)	6(1)					
1N/O	2.48(2)	0(2)	8(2)	0.1471	633.798	35.930	5
3N/O	2.06(1)	4(1)					
2N/O	2.48(2)	4(2)	10(2)	0.1607	692.693	39.269	5
5N/O	2.05(2)	9(1)					
1N/O	2.47(2)	1(2)	7(2)	0.1800	775.831	43.982	5
4N/O	2.06(1)	6(1)					
2N/O	2.48(2)	4(2)	9(2)	0.1450	625.062	35.435	5
3N/O	2.07(1)	4(1)					
3N/O	2.49(3)	10(4)	12(2)	0.1950	840.213	47.632	5
6N/O	2.05(2)	11(2)					
1N/O	2.46(2)	1(2)	6(2)	0.2244	967.059	54.823	5
5N/O	2.06(1)	9(1)					
2N/O	2.47(2)	4(2)	8(2)	0.1616	696.336	39.476	5
4N/O	2.07(1)	6(1)					
3N/O	2.48(2)	9(3)	11(2)	0.1627	701.376	39.761	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**

2S	2.13(2)	5(2)					
1S	2.26(4)	4(3)	neg9(4)	0.2121	914.262	51.830	5
2S	2.11(0.17)	20(17)					
2S	2.16(2)	7(2)	neg13(7)	0.2150	926.659	52.533	5
3S	2.15(3)	10(1)					
1S	2.55(3)	7(4)	neg12(5)	0.2004	863.473	48.951	5
4S	2.14(2)	9(2)					
1S	1.95(5)	10(6)	neg16(4)	0.2155	928.955	52.663	5
3S	2.17(2)	9(1)					
2S	2.43(0.10)	28(22)	neg7(4)	0.2036	877.620	49.753	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.19(2)	11(1)					
2S	2.50(4)	16(7)	neg7(4)	0.1867	804.626	45.615	5
3S	2.41(8)	31(21)					
3S	2.17(2)	9(1)	neg7(5)	0.2033	875.984	49.660	5
6S	2.16(2)	16(2)					
1S	2.97(7)	10(9)	neg12(3)	0.2430	1047.380	59.376	5
5S	2.20(2)	14(1)					
2S	2.51(3)	12(4)	neg7(4)	0.1790	771.289	43.725	5
4S	2.19(2)	11(1)					
3S	2.49(4)	21(7)	neg5(3)	0.1819	783.943	44.442	5

Ni-N(2.0) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.02(3)	4(2)					5
1S	2.23(3)	7(3)	3(4)	0.2108	908.555	51.506	
1N/O	1.89(0.11)	10(10)					5
2S	2.17(2)	6(1)	neg9(5)	0.2181	939.761	53.275	
2N/O	2.03(3)	5(4)					
2S	2.20(4)	11(4)	neg1(5)	0.2169	934.894	53.000	5
3N/O	2.05(3)	6(3)					
1S	2.21(3)	9(6)	5(4)	0.2053	884.958	50.169	5
1N/O	1.94(0.43)	26(50)					
3S	2.16(3)	9(2)	neg10(6)	0.2141	922.777	52.313	5

1N/O 4S			No Fit	No Fit	No Fit	No Fit	5
4N/O 1S	2.07(3) 2.18(5)	9(6) 8(7)	6(4)	0.2046	881.567	49.976	5
2N/O 3S	1.91(0.76) 2.16(3)	53(85) 9(1)	neg10(6)	0.2143	923.519	52.355	5
3N/O 2S	2.05(2) 2.19(3)	6(4) 13(7)	2(4)	0.2113	910.597	51.622	5
5N/O 1S	2.08(4) 2.19(3)	13(6) 6(3)	6(4)	0.2127	916.800	51.974	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.07(3) 2.17(3)	7(3) 14(9)	4(3)	0.2049	883.046	50.060	5
2N/O 4S	2.29(0.30) 2.16(3)	13(53) 11(5)	neg12(8)	0.2184	941.240	53.359	5
3N/O 3S	1.86(0.77) 2.16(3)	66(108) 9(1)	neg10(6)	0.2141	922.717	52.309	5
6N/O 1S	2.08(5) 2.19(2)	17(5) 5(2)	5(4)	0.2261	974.233	55.230	5
1N/O 6S	2.30(7) 2.17(3)	4(6) 16(3)	neg12(5)	0.2545	1096.864	62.182	5
5N/O 2S	2.11(6) 2.17(7)	9(9) 9(5)	6(3)	0.2008	865.555	49.069	5
2N/O 5S	1.58(0.10) 2.15(2)	26(18) 14(1)	neg12(4)	0.2331	1004.691	56.956	5
4N/O 3S	2.06(3) 2.16(3)	7(2) 17(8)	1(4)	0.2124	915.257	51.886	5
3N/O 4S	2.31(0.10) 2.16(3)	12(25) 12(5)	neg14(7)	0.2185	941.861	53.395	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.03(4)	18(4)	5(3)	0.2422	892.375	50.589	5

1Imd	2.04(2)	1(1)					
4N/O	2.04(4)	17(4)					
1Imd	1.55(2)	8(3)					
1Imd	2.05(1)	1(1)	8(2)	0.1583	682.187	43.619	7
3N/O	2.04(3)	8(4)					
1Imd	1.83(3)	2(2)					
1Imd	1.96(3)	4(2)					
1Imd	2.09(3)	3(3)	1(2)	0.1768	762.096	55.874	9
2N/O	2.04(3)	5(3)					
1Imd	2.11(3)	2(3)					
1Imd	1.83(3)	0(3)					
1Imd	1.57(3)	8(4)					
1Imd	1.98(3)	3(3)	6(2)	0.0946	407.786	35.034	11
1N/O	2.04(4)	2(4)					
1Imd	2.15(4)	6(5)					
1Imd	1.93(4)	8(6)					
1Imd	1.82(4)	4(6)					
1Imd	1.59(5)	8(6)					
1Imd	2.04(4)	9(6)	5(3)	0.1180	508.563	52.757	13
4N/O	2.03(4)	14(4)					
1Imd	2.04(2)	1(1)	6(2)	0.2207	951.087	53.918	5
3N/O	2.04(3)	6(3)					
1Imd	2.02(3)	1(2)					
1Imd	1.86(4)	3(3)	3(2)	0.1909	822.598	52.597	7
2N/O	2.04(3)	5(4)					
1Imd	1.97(2)	5(2)					
1Imd	2.10(3)	4(2)					
1Imd	1.84(2	2(2)	2(2)	0.1517	653.809	47.934	9
1N/O	2.04(4)	2(4)					
1Imd	1.86(3)	0(4)					
1Imd	2.00(3)	4(3)					
1Imd	1.56(3)	10(5)					
1Imd	2.12(3)	3(3)	7(2)	0.1193	514.356	44.190	11
0N/O							
1Imd	1.58(6)	12(10)					
1Imd	1.85(4)	4(5)					
1Imd	1.95(4)	9(5)					
1Imd	2.16(3)	7(5)					
1Imd	2.06(3)	9(5)	6(3)	0.1903	820.093	70.457	11
3N/O	2.04(3)	9(3)	7(2)	0.2052	884.493	50.142	5

1Imd	2.04(2)	2(2)					
2N/O	2.05(3)	4(3)					
1Imd	1.90(4)	5(5)					
1Imd	2.04(3)	1(3)	4(2)	0.1925	829.606	53.045	7
1N/O	2.04(4)	2(4)					
1Imd	1.86(2)	3(2)					
1Imd	2.10(2)	5(2)					
1Imd	1.98(2)	6(2)	2(2)	0.1587	683.913	50.142	9
0N/O							
1Imd	1.94(2)	10(3)					
1Imd	2.04(2)	11(3)					
1Imd	1.84(2)	6(3)					
1Imd	2.15(2)	8(3)	2(2)	0.2188	943.009	69.137	9
2N/O	2.06(3)	5(3)					
1Imd	2.04(4)	3(4)	8(2)	0.2067	890.734	50.496	5
1N/O	2.05(4)	2(4)					
1Imd	2.06(7)	3(6)					
1Imd	1.97(9)	6(14)	6(3)	0.2256	972.247	62.166	7
0N/O							
1Imd	1.99(2)	7(2)					
1Imd	2.11(2)	6(2)					
1Imd	1.88(2)	3(2)	3(2)	0.2304	993.020	63.494	7

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O	1.84(2)	1(2)					
1N/O	2.09(2)	9(1)					
1S	2.09(2)	6(1)					
1S	2.25(2)	3(1)	neg6(3)	0.1094	471.361	34.558	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O							
1N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.4)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
1N/O							
1N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(3)	2(2)					
1N/O	2.75(2)	1(2)					
1S	2.24(2)	1(1)					
1S	2.11(2)	1(1)	neg10(4)	0.1123	484.112	35.493	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	1(2)					
1N/O	2.09(2)	8(1)					
1S	2.09(2)	6(1)					
1S	2.25(2)	2(1)	neg7(3)	0.1261	543.465	39.844	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(5)	2(4)					
1N/O	2.02(2)	2(1)					
1S	2.58(4)	9(5)					
1S	2.26(3)	4(2)	1(4)	0.1296	558.569	40.952	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(3)	1(2)					
1N/O	2.10(3)	9(2)					
1S	2.09(2)	6(2)					
1S	2.25(2)	3(2)	neg6(4)	0.1366	588.799	43.168	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(3)	1(2)					
1N/O	2.09(3)	9(2)					
1S	2.09(2)	6(2)					
1S	2.25(2)	2(2)	neg7(4)	0.1392	599.892	43.981	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(4)	2(3)					
1N/O	2.01(2)	2(1)					
1S	2.25(2)	3(2)					
1S	2.59(3)	9(4)	2(3)	0.111	478.209	35.060	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(3)	1(3)					
1N/O	1.98(4)	3(2)					
1S	2.01(0.79)	41(198)					
1S	2.21(5)	2(2)	neg5(16)	0.1488	641.286	47.016	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(4)	2(3)					
1N/O	2.01(2)	2(1)					
1S	2.25(2)	3(2)					
1S	2.59(3)	9(4)	1(3)	0.1143	492.655	36.119	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(4)	2(3)					
1N/O	2.01(2)	2(1)					
1S	2.25(2)	3(2)					
1S	2.58(3)	9(5)	1(4)	0.1169	504.012	36.952	9

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(8)	2(4)					
1N/O	2.12(0.74)	5(217)					
1S	2.11(0.15)	1(5)					
1S	2.24(0.14)	0(10)	neg8(15)	0.1538	662.810	48.594	9

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(4)	1(3)					
1N/O	1.96(6)	2(8)					
1S	2.58(3)	6(4)					
1S	2.28(3)	6(4)	4(4)	0.1375	592.725	43.456	9

Ni-N(1.8) Ni-N(2.1) Ni-S(2.1) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	9

Ni-N(1.8) Ni-N(2.1) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(7)	2(4)					
1N/O	2.12(0.86)	6(215)					
1S	2.11(0.13)	1(4)					
1S	2.23(0.13)	0(9)	neg9(16)	0.1561	672.653	49.316	9

Ni-N(1.8) Ni-N(2.1) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(3)	2(3)					
1N/O	2.01(2)	2(1)					
1S	2.25(2)	3(2)					
1S	2.58(3)	9(4)	1(3)	0.1096	472.346	34.630	9

Ni-N(1.8) Ni-N(2.1) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.82(6)	0(3)					
1N/O	1.98(3)	2(3)					
1S	1.78(7)	13(12)					
1S	2.23(3)	3(3)	1(5)	0.1406	605.814	44.416	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(3)	1(2)					
1N/O	2.09(3)	9(2)					
1S	2.09(3)	6(2)					
1S	2.25(3)	2(2)	neg8(4)	0.1413	608.807	44.635	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.81(3)	1(2)					
1N/O	1.57(6)	11(7)					
1S	2.09(2)	0(1)					
1S	2.22(2)	0(1)	neg12(4)	0.1367	589.256	43.202	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(3)	1(3)					
1N/O	1.98(4)	3(2)					
1S	1.97(0.88)	43(102)					
1S	2.21(4)	2(2)	neg5(12)	0.1482	638.575	46.818	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(4)	2(3)					
1N/O	2.01(2)	2(1)	1(3)	0.1151	496.084	36.371	9

1S	2.25(2)	3(2)					
1S	2.58(3)	9(4)					

Ni-N(1.9) Ni-N(2.0) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(4)	2(3)					
1N/O	2.01(2)	2(1)					
1S	2.25(2)	3(2)					
1S	2.58(3)	9(5)	0(4)	0.1176	506.867	37.161	9

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(8)	2(4)					
1N/O	2.12(0.75)	5(216)					
1S	2.11(0.15)	1(5)					
1S	2.23(0.14)	0(11)	neg8(14)	0.1539	663.127	48.618	9

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(1)					
1N/O	3.03(4)	0(3)					
1S	2.58(4)	9(6)					
1S	2.28(2)	4(2)	7(4)	0.1831	788.943	57.842	9

Ni-N(1.9) Ni-N(2.1) Ni-S(2.1) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(4)	1(3)					
1N/O	1.96(7)	3(8)					
1S	2.58(3)	6(4)					
1S	2.28(4)	6(4)	3(5)	0.1374	592.051	43.407	9

Ni-N(1.9) Ni-N(2.1) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(7)	2(4)					
1N/O	2.12(0.83)	6(205)					
1S	2.11(0.13)	1(4)					
1S	2.23(0.13)	0(9)	neg9(15)	0.1563	673.740	49.396	9

Ni-N(1.9) Ni-N(2.1) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(4)	2(3)					
1N/O	2.01(2)	3(1)					
1S	2.25(2)	3(2)					
1S	2.58(3)	9(4)	0(3)	0.1104	475.961	34.895	9

Ni-N(1.9) Ni-N(2.1) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(3)	9(2)					
1N/O	1.84(3)	1(2)					
1S	2.09(3)	6(2)					
1S	2.25(3)	3(2)	neg7(4)	0.145	624.823	45.809	9

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(6)	2(3)					
1N/O	2.13(0.64)	4(138)					
1S	2.10(9)	1(5)					
1S	2.23(0.13)	0(9)	neg9(10)	0.1555	670.256	49.140	9

Ni-N(2.0) Ni-N(2.1) Ni-S(2.1) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.81(3)	1(2)					
1N/O	1.57(6)	11(7)					
1S	2.09(2)	1(1)					
1S	2.22(2)	0(1)	neg12(4)	0.1378	594.064	43.554	9

Ni-N(2.0) Ni-N(2.1) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(7)	2(5)					
1N/O	2.12(0.84)	6(206)					
1S	2.11(0.13)	1(4)					
1S	2.23(0.13)	0(9)	neg9(15)	0.1585	683.275	50.095	9

Ni-N(2.0) Ni-N(2.1) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(6)	2(4)					
1N/O	2.13(0.85)	5(170)					
1S	2.10(0.11)	1(4)					
1S	2.23(0.13)	0(8)	neg10(13)	0.1586	683.711	50.127	9

Ni-N(2.0) Ni-N(2.1) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	2(2)					
1N/O	1.91(4)	2(4)					
1S	2.25(2)	4(2)	0(3)	0.1197	515.661	37.806	9

1S	2.58(3)	8(4)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(3)	1(3)					
1N/O	2.23(0.51)	10(51)					
1S	2.11(2)	2(2)					
1S	2.24(3)	1(2)					
1C	2.78(3)	2(2)	neg10(7)	0.1033	445.150	38.244	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	1(1)					
1N/O	2.09(1)	9(1)					
1S	2.10(1)	6(1)					
1S	2.26(1)	3(1)					
2C	2.88(5)	7(6)	neg5(2)	0.0675	290.752	24.979	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(1)					
1N/O	2.09(1)	9(1)					
1S	2.10(1)	6(1)					
1S	2.26(1)	3(1)					
3C	2.89(4)	10(5)	neg5(2)	0.0594	255.947	21.989	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	1(1)					
1N/O	2.10(1)	9(1)					
1S	2.10(1)	6(1)					
1S	2.26(1)	3(1)					
4C	2.89(4)	12(5)	neg5(2)	0.0555	239.391	20.567	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(3)	1(3)					
1N/O	2.23(0.51)	10(50)					
1S	2.10(2)	2(2)					
1S	2.24(3)	1(2)					
1C	2.78(3)	2(2)	neg10(7)	0.1033	445.151	38.244	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	1(1)					
1N/O	2.09(1)	9(1)					
1S	2.10(1)	6(1)					
1S	2.26(1)	3(1)					
2C	2.88(5)	7(6)	neg5(2)	0.0668	287.941	24.738	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(1)					
1N/O	2.09(1)	9(1)					
1S	2.10(1)	6(1)					
1S	2.26(1)	3(1)					
3C	2.89(4)	10(5)	neg5(2)	0.0589	253.672	21.794	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	1(1)					
1N/O	2.10(1)	9(1)					
1S	2.10(1)	6(1)					
1S	2.26(1)	3(1)					
4C	2.89(4)	12(5)	neg5(2)	0.0553	238.249	20.469	11

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.4) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	0(2)					
1N/O	1.98(2)	3(1)					
1S	2.22(2)	2(1)					
1S	1.98(0.35)	37(44)					
4C	2.91(8)	14(8)	neg3(5)	0.1019	439.248	37.737	11

Ni-N(1.8) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	1(2)					
1N/O	1.98(2)	4(1)					
1S	2.22(2)	2(1)					
1S	1.90(0.23)	30(25)					
4C	2.92(7)	14(7)	neg3(4)	0.0935	402.835	34.609	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(4)	1(2)					
1N/O	1.98(2)	3(2)	neg1(3)	0.0916	394.842	33.922	11

1S	2.22(2)	2(2)					
1S	1.82(8)	17(15)					
4C	2.94(7)	15(8)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	0(2)					
1N/O	2.11(3)	6(3)					
1S	2.11(2)	4(2)					
1S	2.26(2)	0(2)					
4C	2.87(3)	9(4)					
0.5Imd	2.00(2)	2(2)	neg4(2)	0.0497	214.333	22.234	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	0(2)					
1N/O	2.11(3)	6(3)					
1S	2.11(2)	3(2)					
1S	2.26(2)	0(2)					
4C	2.87(3)	8(4)					
0.7Imd	2.00(2)	1(2)	neg4(2)	0.0558	240.675	24.967	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(2)	0(2)					
1N/O	2.11(3)	6(2)					
1S	2.10(2)	4(2)					
1S	2.26(2)	1(2)					
4C	2.87(4)	9(5)					
1Imd	2.00(3)	2(3)	neg4(2)	0.0662	285.482	29.615	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	3(2)					
1N/O	2.39(1)	1(1)					
2S	2.20(2)	11(2)					
4C	2.86(2)	6(2)					
1Cl	3.92(2)	3(2)					
0.5Imd	2.00(1)	4(1)	neg6(1)	0.0279	102.761	10.660	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	3(2)	neg6(1)	0.027	116.500	12.086	13

1N/O	2.39(1)	1(1)
2S	2.20(2)	11(2)
4C	2.85(2)	6(2)
1Cl	3.92(2)	3(2)
0.5Imd	2.00(1)	4(1)

Ni-N(1.8) Ni-N(1.9) Ni-S(2.3) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	3(2)					
1N/O	2.39(1)	1(1)					
2S	2.21(2)	12(2)					
4C	2.85(2)	6(2)					
1Cl	3.92(2)	3(2)					
0.5Imd	2.00(1)	4(1)	neg7(1)	0.0264	113.585	11.783	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	3(2)					
1N/O	2.39(1)	1(1)					
2S	2.20(2)	11(2)					
4C	2.86(2)	6(2)					
1Cl	3.92(2)	3(2)					
0.5Imd	2.00(1)	4(1)	neg6(1)	0.0278	119.792	12.427	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	2(1)					
1N/O	2.39(1)	1(1)					
2S	2.21(2)	11(2)					
4C	2.86(1)	3(1)					
1Cl	3.92(2)	3(2)					
0.5Imd	2.00(1)	4(1)	neg6(1)	0.0241	103.940	10.783	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	2(1)					
1N/O	2.39(1)	1(1)					
2S	2.21(2)	11(2)					
4C	2.85(1)	3(1)					
1Cl	3.92(2)	3(2)					
0.5Imd	2.00(1)	4(1)	neg6(1)	0.024	103.569	10.744	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	3(2)					
1N/O	2.39(1)	1(1)					
2S	2.20(2)	11(2)					
4C	2.86(2)	6(2)					
1Cl	3.92(2)	3(2)					
0.5Imd	2.00(1)	4(1)	neg6(1)	0.0281	120.925	12.545	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	3(2)					
1N/O	2.39(1)	1(1)					
2S	2.20(2)	11(2)					
4C	2.86(2)	6(2)					
1Cl	3.92(2)	2(2)					
0.5Imd	2.00(1)	4(1)	neg6(1)	0.0272	117.211	12.159	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	2(1)					
1N/O	2.39(1)	1(1)					
2S	2.21(2)	11(2)					
3C	2.85(1)	3(1)					
1Cl	3.92(2)	2(2)					
0.5Imd	2.00(1)	4(1)	neg6(2)	0.0253	109.044	11.312	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(2)	2(1)					
1N/O	2.39(1)	1(1)					
2S	2.21(2)	11(2)					
3C	2.85(2)	3(1)					
1Cl	3.92(2)	2(2)					
0.5Imd	2.00(1)	4(1)	neg6(2)	0.0258	111.035	11.519	13

Ni-N(1.8) Ni-N(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.93(5)	12(7)					
1S	2.08(3)	6(4)					
1S	2.24(1)	2(1)					
4C	2.86(2)	6(2)					
1Cl	3.93(2)	3(2)					
0.5Imd	2.01(1)	4(1)	neg5(2)	0.0474	204.153	21.178	13

Ni-N(1.9) Ni-N(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.95(5)	13(8)					
1S	2.08(3)	6(4)					
1S	2.24(1)	2(1)					
4C	2.86(2)	6(2)					
1Cl	3.93(2)	3(2)					
0.5Imd	2.00(1)	4(1)	neg5(2)	0.0495	213.374	22.135	13

Ni-N(2.0) Ni-N(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(6)	13(10)					
1S	2.08(3)	6(4)					
1S	2.23(1)	2(1)					
4C	2.86(2)	6(2)					
1Cl	3.93(3)	3(2)					
0.5Imd	2.00(1)	4(1)	neg5(2)	0.0515	221.995	23.029	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.12(6)	4(3)					
1S	2.11(3)	2(2)					
1S	2.24(2)	0(2)					
4C	2.87(2)	9(3)					
1Cl	3.95(3)	5(3)					
0.25Imd	2.01(1)	5(1)	neg5(1)	0.0239	103.209	13.510	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.13(6)	4(3)					
1S	2.11(3)	2(2)					
1S	2.24(2)	0(2)					
4C	2.87(2)	9(3)					
1Cl	3.95(3)	5(3)					
0.25Imd	2.01(1)	5(1)	neg5(1)	0.0241	103.936	13.605	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.12(5)	4(3)					
1S	2.11(3)	2(2)					
1S	2.25(2)	0(2)	neg5(1)	0.024	103.548	13.554	15

4C	2.87(2)	8(3)					
1Cl	3.95(3)	5(3)					
0.25Imd	2.01(1)	5(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.13(6)	4(3)					
1S	2.11(3)	2(2)					
1S	2.24(2)	0(2)					
4C	2.87(2)	9(3)					
1Cl	3.95(3)	5(3)					
0.25Imd	2.01(1)	5(1)	neg5(1)	0.0237	102.343	13.396	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(5)	2(16)					
1N/O	2.05(8)	4(4)					
1S	2.06(6)	1(8)					
1S	2.24(2)	1(2)					
4C	2.92(4)	11(5)					
1Cl	4.01(4)	6(4)					
0.25Imd	1.78(1)	5(1)	neg5(2)	0.0399	172.020	22.517	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(6)	2(16)					
1N/O	2.00(5)	3(2)					
1S	2.03(7)	3(13)					
1S	2.23(2)	0(2)					
4C	2.86(3)	8(3)					
1Cl	3.95(3)	4(3)					
0.25Imd	2.01(1)	6(1)	neg5(2)	0.0342	147.550	19.314	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.14(6)	3(3)					
1S	2.12(4)	1(3)					
1S	2.24(2)	1(3)					
4C	2.86(2)	8(2)					
1Cl	3.94(3)	5(3)					
0.25Imd	2.00(1)	5(1)	neg6(1)	0.0237	102.229	13.381	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.15(6)	3(3)					
1S	2.12(5)	1(3)					
1S	2.23(3)	1(4)					
4C	2.86(2)	7(2)					
1Cl	3.94(2)	4(3)					
0.4Imd	2.00(1)	4(1)	neg5(1)	0.0236	101.854	13.332	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.15(6)	3(3)					
1S	2.12(5)	1(3)					
1S	2.23(3)	1(4)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	3(3)					
0.4Imd	2.00(1)	4(1)	neg5(1)	0.0237	102.354	13.398	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.15(6)	3(3)					
1S	2.12(5)	1(3)					
1S	2.24(3)	1(4)					
4C	2.86(2)	7(2)					
1Cl	3.94(2)	4(3)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.0237	102.090	13.363	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.15(6)	3(3)					
1S	2.12(5)	1(3)					
1S	2.24(3)	1(4)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	4(3)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.0238	102.599	13.430	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.15(6)	3(3)	neg6(1)	0.0234	100.896	13.207	15

1S	2.12(5)	0(3)					
1S	2.23(3)	1(5)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	4(2)					
0.4Imd	2.00(1)	4(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.15(6)	3(3)					
1S	2.12(5)	0(4)					
1S	2.23(3)	1(5)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	3(2)					
0.4Imd	2.00(1)	4(1)	neg6(1)	0.0235	101.390	13.272	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.16(6)	3(3)					
1S	2.23(3)	1(5)					
1S	2.13(5)	1(4)					
4C	2.87(2)	8(2)					
1Cl	3.94(2)	4(2)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.0215	92.473	12.104	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	1(2)					
1N/O	2.16(5)	4(3)					
1S	2.23(4)	1(5)					
1S	2.13(5)	1(4)					
4C	2.86(2)	8(2)					
1Cl	3.94(2)	4(2)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.021	90.607	11.860	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(3.0) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	1(2)					
1N/O	2.16(5)	4(3)					
1S	2.23(4)	1(5)					
1S	2.13(5)	1(4)					
4C	2.86(2)	8(2)					
1Cl	3.94(2)	3(2)	neg5(1)	0.0211	91.072	11.921	15

0.4Imd	2.01(1)	4(1)					

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	0(1)					
1N/O	2.15(4)	4(2)					
1S	2.24(2)	1(3)					
1S	2.13(3)	2(3)					
4C	2.87(2)	8(2)					
1Cl	3.94(2)	4(2)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.0189	81.521	10.671	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(3.0) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	1(2)					
1N/O	2.17(3)	4(2)					
1S	2.15(9)	1(3)					
1S	2.21(8)	4(11)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	4(2)					
0.4Imd	2.01(1)	4(1)	neg6(1)	0.0206	88.925	11.640	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(3.0) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(1)	0(1)					
1N/O	2.15(4)	4(2)					
1S	2.24(2)	1(3)					
1S	2.13(3)	2(3)					
4C	2.87(2)	8(2)					
1Cl	3.94(2)	3(2)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.019	81.993	10.733	15

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	0(1)					
1N/O	2.15(5)	4(2)					
1S	2.24(2)	1(3)					
1S	2.13(3)	2(3)					
4C	2.87(2)	8(2)					
1Cl	3.94(2)	3(2)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.0195	84.170	11.017	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(3.0) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	1(1)					
1N/O	2.12(2)	5(2)					
1S	2.25(1)	1(1)					
1S	2.11(1)	4(2)					
4C	2.87(2)	8(2)					
1Cl	3.95(2)	5(3)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.0174	75.068	9.826	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(3.0) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	0(1)					
1N/O	2.12(2)	6(2)					
1S	2.25(1)	1(1)					
1S	2.11(2)	4(2)					
4C	2.87(2)	8(2)					
1Cl	3.94(2)	4(3)					
0.4Imd	2.01(1)	4(1)	neg5(1)	0.0176	75.873	9.931	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.17(2)	3(2)					
1S	2.15(0.11)	1(4)					
1S	2.21(9)	4(11)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	4(2)					
0.4Imd	2.00(1)	4(1)	neg6(2)	0.0234	100.735	13.186	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.17(2)	3(2)					
1S	2.15(0.11)	1(4)					
1S	2.21(0.10)	4(11)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	3(2)					
0.4Imd	2.00(1)	4(1)	neg6(2)	0.0235	101.160	13.242	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.17(2)	3(2)					
1S	2.16(0.12)	2(5)	neg6(2)	0.0232	99.956	13.084	15

1S	2.20(0.12)	4(12)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	4(2)					
0.4Imd	2.00(1)	4(1)					

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.17(2)	3(2)					
1S	2.16(0.12)	2(5)					
1S	2.20(0.11)	4(12)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	3(2)					
0.4Imd	2.00(1)	4(1)	neg6(2)	0.0233	100.383	13.140	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	0(2)					
1N/O	2.11(4)	5(3)					
1S	2.11(2)	3(2)					
1S	2.26(2)	0(2)					
4C	2.87(3)	8(4)					
1Cl	3.43(0.16)	23(28)					
0.5Imd	2.01(2)	2(2)	neg4(2)	0.0458	197.266	25.821	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	0(2)					
1N/O	2.11(4)	5(3)					
1S	2.11(2)	3(2)					
1S	2.26(2)	0(2)					
4C	2.87(3)	8(4)					
1Cl	3.43(0.16)	23(28)					
0.5Imd	2.01(2)	2(2)	neg4(2)	0.0458	197.175	25.809	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(2)	1(2)					
1N/O	2.17(4)	3(3)					
1S	2.14(9)	1(6)					
1S	2.22(7)	2(9)					
4C	2.86(2)	7(2)					
1Cl	3.93(2)	4(2)					
0.5Imd	2.00(1)	4(1)	neg5(1)	0.0236	101.723	13.315	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	1(1)					
1N/O	2.15(6)	3(4)					
1S	2.12(5)	0(3)					
1S	2.23(3)	1(4)					
4C	2.86(2)	7(2)					
2Cl	3.95(2)	8(3)					
0.5Imd	2.01(1)	3(1)	neg6(1)	0.0221	95.275	12.471	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	0(1)					
1N/O	2.13(6)	4(3)					
1S	2.24(2)	0(2)					
1S	2.12(3)	2(2)					
4C	2.87(2)	7(2)					
1Cl	3.93(2)	4(2)					
0.5Imd	2.01(1)	4(1)	neg5(1)	0.021	90.580	11.857	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(1)	1(1)					
1N/O	2.15(6)	3(4)					
1S	2.12(5)	0(3)					
1S	2.23(3)	1(4)					
4C	2.86(2)	7(2)					
2Cl	3.95(2)	9(3)					
0.5Imd	2.01(1)	3(1)	neg6(1)	0.0221	95.196	12.461	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(1)	1(1)					
1N/O	2.15(7)	3(3)					
1S	2.24(3)	1(4)					
1S	2.12(5)	1(3)					
4C	2.86(2)	6(2)					
1Cl	3.92(2)	3(2)					
0.7Imd	2.01(1)	3(1)	neg5(1)	0.0221	95.395	12.487	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.84(2)	1(1)					
1N/O	2.18(3)	3(2)					
1S	2.18(8)	8(10)					
1S	2.18(5)	2(5)					
4C	2.85(2)	5(2)					
2Cl	3.92(2)	2(2)					
1Imd	2.00(1)	2(1)	neg5(1)	0.0261	112.688	14.750	15

Table I.3. Additional Fits for Oxidized H53A-NiSOD in Buffer with 50 mM Tris, 100 mM NaCl and 10 % Glycerol at pH 8.0.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	1(1)	8(3)	0.1994	828.240	42.172	3
3N/O	2.09(1)	1(1)	7(2)	0.1522	632.086	32.184	3
4N/O	2.09(1)	2(1)	6(2)	0.1520	631.317	32.145	3
5N/O	2.09(1)	4(1)	5(2)	0.1787	742.257	37.794	3
6N/O	2.09(1)	6(1)	4(2)	0.2193	910.559	46.363	3
7N/O	2.08(2)	8(1)	4(2)	0.2649	1099.996	56.009	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.18(1)	3(1)	neg14(4)	0.2348	975.143	49.652	3
3S	2.18(2)	6(1)	neg15(4)	0.2369	983.957	50.101	3
4S	2.18(2)	8(1)	neg16(4)	0.2554	1060.595	54.003	3
5S	2.18(2)	10(1)	neg16(4)	0.2773	1151.368	58.625	3
6S	2.18(2)	12(1)	neg16(4)	0.2987	1240.381	63.157	3
7S	2.18(3)	14(2)	neg16(4)	0.3187	1323.574	67.393	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.09(1)	3(1)					
1N/O	1.97(2)	2(1)	2(2)	0.1060	440.345	24.963	5
2N/O	2.09(1)	2(1)					
2N/O	1.98(1)	1(1)	0(2)	0.0856	355.644	20.162	5
3N/O	2.08(1)	1(0)					
1N/O	1.94(1)	2(1)	1(2)	0.0794	329.782	18.694	5
4N/O	2.07(1)	0(0)					
1N/O	1.92(1)	2(1)	1(1)	0.0792	328.820	18.641	5
3N/O	2.09(1)	1(1)					
2N/O	1.95(1)	1(1)	neg1(2)	0.0840	348.827	19.775	5
5N/O	2.07(1)	2(1)	0(1)	0.0969	402.390	22.812	5

1N/O	1.90(1)	1(1)					
4N/O	2.08(1)	0(1)					
2N/O	1.93(1)	2(1)	neg1(2)	0.0978	406.015	23.017	5
3N/O	2.09(1)	0(1)					
3N/O	1.96(2)	4(2)	neg2(2)	0.1002	416.192	23.594	5
6N/O							
1N/O			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.09(1)	4(1)					
2N/O	1.59(0.14)	59(54)	6(3)	0.1699	705.602	40.001	5
4N/O	2.10(1)	2(1)					
3N/O	2.38(6)	21(13)	8(2)	0.1414	587.244	33.291	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.20(1)	2(1)					
1S	2.37(2)	2(2)	neg7(3)	0.1571	652.442	36.987	5
2S	2.10(1)	2(1)					
2S	2.36(2)	7(2)	neg7(3)	0.1473	611.590	34.671	5
3S	2.21(1)	4(1)					
1S	2.40(1)	1(1)	neg8(2)	0.1361	565.191	32.041	5
4S	2.18(2)	8(1)					
1S	3.45(0.10)	7(11)	neg16(4)	0.2405	998.667	56.615	5
3S	2.20(1)	4(1)					
2S	2.39(2)	5(2)	neg7(2)	0.1432	594.509	33.703	5
5S	2.18(2)	10(1)					
1S	2.94(8)	9(10)	neg15(4)	0.2539	1054.160	59.761	5
4S	2.21(1)	6(1)					
2S	2.41(2)	5(1)	neg8(2)	0.1518	630.217	35.727	5
3S	2.20(1)	4(1)					
3S	2.39(2)	9(2)	neg7(2)	0.1495	620.622	35.183	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.21(1)	8(1)					
2S	2.42(2)	4(1)	neg9(2)	0.1677	696.423	39.481	5

4S	2.20(1)	6(1)					
3S	2.41(2)	8(2)	neg8(2)	0.1639	680.514	38.579	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.93(4)	5(3)					5
1S	2.18(1)	0(1)	neg14(5)	0.1830	759.843	43.076	
1N/O	1.87(2)	1(2)					5
2S	2.17(1)	3(1)	neg18(3)	0.1756	729.285	41.344	
2N/O	1.88(4)	7(4)					
2S	2.17(1)	3(1)	neg17(4)	0.1840	764.199	43.323	5
3N/O	1.94(5)	9(4)					
1S	2.18(1)	0(1)	neg13(5)	0.1753	727.928	41.267	5
1N/O	1.35(3)	5(3)					
3S	2.18(2)	6(1)	neg16(4)	0.2169	900.661	51.059	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	1.96(6)	13(4)					
1S	2.19(1)	0(1)	neg12(6)	0.1704	707.517	40.109	5
2N/O	1.84(5)	9(6)					
3S	2.17(2)	5(1)	neg18(4)	0.2091	868.227	49.220	5
3N/O	1.88(5)	12(6)					
2S	2.18(1)	3(1)	neg17(4)	0.1861	772.995	43.821	5
5N/O	2.16(2)	4(3)					
1S	2.19(2)	0(1)	8(2)	0.1363	565.871	32.079	5
1N/O	3.76(0.33)	6(37)					
5S	2.18(2)	10(1)	neg16(4)	0.2743	1138.959	64.568	5
4N/O	1.88(6)	17(8)					
2S	2.18(2)	3(1)	neg17(5)	0.1859	772.073	43.769	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
3N/O	1.23(0.18)	31(36)					
3S	2.18(2)	6(1)	neg15(4)	0.2283	948.214	53.755	5
6N/O	2.17(2)	7(2)					
1S	2.20(1)	0(1)	8(2)	0.1211	503.015	28.516	5

1N/O	2.30(1)	4(0)					
6S	2.23(2)	12(1)	neg12(3)	0.0979	406.513	23.045	5
5N/O	1.88(7)	20(9)					
2S	2.18(2)	3(1)	neg17(5)	0.1854	769.844	43.643	5
2N/O	2.65(0.11)	10(15)					
5S	2.19(2)	10(1)	neg15(4)	0.2606	1082.145	61.347	5
4N/O	1.83(6)	18(10)					
3S	2.17(2)	5(1)	neg18(4)	0.2094	869.470	49.289	5
3N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	3(1)					
1Imd	1.91(3)	3(3)	2(2)	0.1501	623.427	35.342	5
4N/O	2.10(1)	3(1)					
1Imd	2.05(2)	2(1)					
1Imd	1.91(2)	1(1)	2(1)	0.0931	386.533	24.715	7
3N/O	2.09(1)	1(1)					
1Imd	2.05(2)	2(2)					
1Imd	1.92(2)	1(1)					
1Imd	2.68(0.14)	14(21)	2(1)	0.0739	306.960	22.505	9
2N/O	2.10(1)	1(1)					
1Imd	1.96(2)	4(1)					
1Imd	2.23(3)	4(3)					
1Imd	2.09(3)	6(2)					
1Imd	2.38(7)	6(11)	6(2)	0.0488	202.774	17.421	11
1N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	13
4N/O	2.09(1)	2(1)					
1Imd	1.95(3)	3(3)	3(2)	0.1198	497.657	28.212	5
3N/O	2.10(1)	1(1)					
1Imd	2.05(2)	2(1)					
1Imd	1.92(1)	1(1)	2(1)	0.0787	326.655	20.886	7

2N/O	2.10(1)	1(1)					
1Imd	2.22(3)	2(2)					
1Imd	1.95(2)	4(1)					
1Imd	2.08(2)	5(1)	5(1)	0.0519	215.347	15.788	9
1N/O	2.10(1)	3(1)					
1Imd	1.96(2)	5(2)					
1Imd	2.27(0.17)	14(48)					
1Imd	2.20(5)	4(4)					
1Imd	2.08(3)	6(3)	6(2)	0.0656	272.257	23.390	11
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
3N/O	2.10(1)	0(1)					
1Imd	1.98(3)	3(3)	4(2)	0.1030	427.528	24.237	5
2N/O	2.09(1)	1(1)					
1Imd	2.07(2)	1(2)					
1Imd	1.94(2)	0(2)	3(2)	0.0838	348.148	22.261	7
1N/O	2.09(1)	3(1)					
1Imd	1.96(2)	5(1)					
1Imd	2.21(2)	4(2)					
1Imd	2.08(2)	6(2)	6(2)	0.0691	286.943	21.037	9
0N/O							
1Imd	2.18(4)	8(4)					
1Imd	2.26(0.11)	3(21)					
1Imd	1.97(3)	7(3)					
1Imd	2.08(3)	9(3)	8(3)	0.2187	908.313	66.594	9
2N/O	2.10(1)	1(1)					
1Imd	2.01(3)	2(2)	5(2)	0.1147	476.487	27.012	5
1N/O	2.10((1)	4(1)					
1Imd	1.98(3)	0(2)					
1Imd	2.11(4)	0(4)	4(2)	0.1154	479.039	30.630	7
0N/O							
1Imd	1.97(2)	6(2)					
1Imd	2.19(2)	7(2)					
1Imd	2.08(2)	9(2)	6(2)	0.2358	979.155	62.607	7

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	4(1)					
1N/O	2.08(1)	6(1)					
1S	2.47(9)	10(10)					
1S	2.29(4)	3(3)	2(3)	0.0783	325.239	23.845	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(5)	1(5)					
1N/O	1.88(0.16)	8(18)					
1S	2.33(4)	0(2)					
1S	2.19(3)	3(1)	neg8(6)	0.0924	383.71	28.132	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(4)	1(3)					
1N/O	1.85(0.13)	8(16)					
1S	2.18(2)	3(1)					
1S	2.32(4)	1(2)	neg9(5)	0.0863	358.489	26.283	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(0.16)	10(19)					
1N/O	1.95(4)	1(3)					
1S	2.19(2)	3(1)					
1S	2.33(4)	1(2)	neg8(5)	0.0856	355.52	26.065	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.85(0.15)	10(18)					
1N/O	1.94(3)	1(3)					
1S	2.18(2)	2(1)					
1S	2.33(4)	1(2)	neg9(5)	0.0845	350.926	25.725	9

Ni-N(1.8) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(0.15)	10(18)					
1N/O	1.95(4)	1(3)					
1S	2.19(2)	2(1)					
1S	2.33(4)	1(2)	neg9(5)	0.087	361.418	26.498	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(3)	1(4)					
1N/O	1.87(0.15)	10(20)					
1S	2.18(2)	2(1)					
1S	2.33(4)	1(2)	neg9(5)	0.0836	347.072	25.446	9

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	4(1)					
1N/O	2.08(1)	6(1)					
1S	2.31(3)	3(2)					
1S	2.53(7)	12(9)	1(3)	0.0677	281.298	20.624	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	4(4)					
1S	2.20(1)	1(1)					
1S	2.36(3)	2(2)					
1Imd	1.90(9)	10(10)	neg7(3)	0.0746	309.607	22.699	9

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(3)	1(2)					
1N/O	2.51(3)	3(2)					
1S	2.98(6)	6(7)					
1S	2.19(1)	1(1)					
1C	2.70(6)	1(5)	neg11(3)	0.091	378.055	32.48	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(4)	0(3)					
1N/O	1.92(0.18)	11(23)					
1S	2.19(1)	2(1)					
1S	2.34(2)	1(2)					
2C	2.87(6)	8(7)	neg6(3)	0.0558	231.744	19.91	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	3(1)					
1N/O	2.06(2)	5(1)					
1S	2.39(4)	4(4)					
1S	2.24(3)	1(3)					
3C	2.94(5)	9(5)	neg2(2)	0.0426	176.763	15.186	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	3(1)					
1N/O	2.06(2)	4(1)					
1S	2.38(3)	3(4)					
1S	2.23(3)	1(3)					
4C	2.94(4)	11(5)	neg2(2)	0.0383	159.143	13.672	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(4)	1(4)					
1N/O	1.90(0.17)	11(23)					
1S	2.19(2)	2(1)					
1S	2.33(3)	1(2)					
1C	2.86(8)	5(9)	neg7(4)	0.0667	277.136	23.81	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	3(1)					
1N/O	2.06(2)	5(1)					
1S	2.40(5)	6(6)					
1S	2.25(4)	2(4)					
2C	2.95(5)	7(6)	neg1(2)	0.0492	204.277	17.55	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	3(1)					
1N/O	2.06(2)	5(1)					
1S	2.39(4)	4(4)					
1S	2.24(3)	1(3)					
3C	2.94(5)	9(5)	neg2(2)	0.0422	175.127	15.046	11

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	3(1)					
1N/O	2.06(2)	4(2)					
1S	2.38(3)	3(3)					
1S	2.23(3)	0(3)					
4C	2.94(4)	11(5)	neg2(2)	0.038	157.665	13.546	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	4(1)					
1N/O	2.08(1)	6(1)					
1S	2.47(8)	11(10)					
1S	2.29(3)	3(3)					
1C	2.98(7)	4(7)	1(3)	0.0532	220.927	18.981	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	4(1)					
1N/O	2.08(1)	6(1)					
1S	2.28(3)	3(3)					
1S	2.46(8)	13(10)					
2C	2.98(5)	7(5)	0(2)	0.0421	174.855	15.022	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	4(1)					
1N/O	2.07(1)	6(1)					
1S	2.27(3)	4(3)					
1S	2.43(9)	13(11)					
3C	2.97(4)	9(5)	neg1(2)	0.0375	155.877	13.392	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	3(1)					
1N/O	2.07(1)	5(1)					
1S	2.25(4)	4(4)					
1S	2.39(9)	12(12)					
4C	2.96(4)	11(5)	neg2(2)	0.0351	145.781	12.524	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	4(1)					
1N/O	2.08(1)	6(1)					
1S	2.47(8)	11(10)					
1S	2.29(3)	3(3)					
1C	2.98(7)	4(7)	1(3)	0.053	220.047	18.905	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	4(1)					
1N/O	2.08(1)	5(1)	0(2)	0.0435	180.514	15.509	11

1S	2.45(8)	11(10)					
1S	2.28(3)	3(3)					
2C	2.97(5)	7(5)					

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	4(1)					
1N/O	2.07(1)	5(1)					
1S	2.42(8)	11(10)					
1S	2.27(3)	4(4)					
3C	2.96(4)	9(5)	neg1(2)	0.0381	158.401	13.609	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	3(1)					
1N/O	2.07(1)	5(1)					
1S	2.25(4)	4(4)					
1S	2.39(8)	12(12)					
4C	2.95(4)	11(5)	neg2(2)	0.0349	145.074	12.464	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	4(1)					
1N/O	2.07(1)	5(1)					
1S	2.27(3)	4(3)					
1S	2.44(8)	13(10)					
3C	2.97(4)	9(5)	neg1(2)	0.0377	156.753	13.467	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	3(1)					
1N/O	2.07(1)	5(1)					
1S	2.26(4)	4(4)					
1S	2.41(8)	12(11)					
4C	2.96(4)	11(4)	neg2(2)	0.0352	146.214	12.562	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	4(1)					
1N/O	2.07(1)	6(1)					
1S	2.27(3)	4(3)					
1S	2.44(8)	13(10)					
3C	2.97(4)	9(5)	neg1(2)	0.0375	155.877	13.392	11

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.9)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(1)	3(1)					
1N/O	2.07(1)	5(1)					
1S	2.26(4)	4(4)					
1S	2.40(8)	12(11)					
4C	2.95(4)	11(4)	neg2(2)	0.035	145.471	12.498	11

Ni-N(1.8) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(2)	6(2)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.89(3)	10(4)					
0.5Imd	2.01(3)	1(3)	neg4(2)	0.0336	139.716	12.003	11

Ni-N(1.8) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	7(3)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.88(3)	10(4)					
0.7Imd	2.00(3)	2(3)	neg4(2)	0.033	137.071	11.776	11

Ni-N(1.8) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(5)	5(6)					
1S	1.70(7)	22(12)					
1S	2.27(7)	12(11)					
4C	2.95(4)	6(5)					
1Imd	2.08(2)	1(1)	1(3)	0.124	514.913	44.238	11

Ni-N(1.8) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(3)	7(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.88(3)	9(4)					
0.5Imd	2.00(3)	0(3)	neg5(1)	0.0332	137.863	11.844	11

Ni-N(1.8) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	7(3)	neg4(2)	0.0351	145.865	12.532	11

1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.88(3)	10(4)					
0.7Imd	2.00(4)	2(3)					

Ni-N(1.8) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(4)	9(4)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.87(1)	9(4)					
1Imd	2.00(3)	3(3)	neg4(2)	0.0337	139.985	12.027	11

Ni-N(1.8) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(3)	7(3)					
1S	2.21(1)	1(0)					
1S	2.36(1)	1(1)					
4C	2.88(3)	9(4)					
0.5Imd	2.00(3)	0(3)	neg5(1)	0.0343	142.256	12.222	11

Ni-N(1.8) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	8(3)					
1S	2.21(1)	1(0)					
1S	2.36(1)	1(1)					
4C	2.87(3)	9(4)					
0.7Imd	1.99(3)	2(3)	neg5(1)	0.034	141.036	12.117	11

Ni-N(1.8) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(4)	11(5)					
1S	2.21(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
1Imd	1.99(3)	3(3)	neg5(1)	0.0332	137.819	11.84	11

Ni-N(1.9) Ni-S(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(4)	0(4)					
1N/O	1.98(0.46)	23(49)					
1S	2.20(2)	2(1)					
1S	2.35(3)	1(2)					
1Imd	1.91(9)	9(11)	neg7(5)	0.0744	308.871	26.536	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	6(3)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.88(3)	9(4)					
0.5Imd	2.00(4)	1(3)	neg5(2)	0.0333	138.167	11.87	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(4)	2(2)					
1S	2.32(4)	4(6)					
1S	2.14(4)	1(9)					
4C	2.90(6)	11(8)					
0.7Imd	1.97(4)	0(2)	neg2(3)	0.0886	367.888	31.606	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(3)	3(2)					
1S	2.12(3)	1(5)					
1S	2.31(3)	3(4)					
4C	2.87(4)	9(6)					
1Imd	1.98(4)	1(2)	neg3(2)	0.0638	265.018	22.769	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(3)	7(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.88(3)	9(4)					
0.5Imd	2.00(3)	0(3)	neg5(1)	0.0334	138.659	11.913	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	8(3)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.87(3)	9(4)					
0.7Imd	2.00(3)	2(3)	neg5(2)	0.0341	141.695	12.174	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	10(5)	neg5(2)	0.0334	138.553	11.904	11

1S	2.36(1)	1(1)					
1S	2.21(1)	1(0)					
4C	2.87(3)	9(4)					
1Imd	2.00(3)	3(3)					

Ni-N(1.9) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(3)	7(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.88(3)	9(4)					
0.5Imd	2.00(3)	0(3)	neg5(1)	0.0335	139.321	11.969	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(1)	1(1)					
1S	1.72(6)	21(8)					
1S	2.30(0.10)	20(16)					
4C	3.00(0.11)	18(15)					
0.7Imd	1.99(5)	2(4)	2(3)	0.0881	365.685	31.417	11

Ni-N(1.9) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	10(5)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.87(3)	9(4)					
1Imd	1.99(3)	3(3)	neg5(2)	0.0341	141.418	12.15	11

Ni-N(1.9) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	7(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.5Imd	2.00(4)	1(3)	neg5(1)	0.0343	142.441	12.238	11

Ni-N(1.9) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(4)	9(4)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.7Imd	1.99(3)	2(3)	neg5(1)	0.0337	139.942	12.023	11

Ni-N(1.9) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(5)	13(6)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.86(3)	8(3)					
1Imd	1.99(3)	3(3)	neg5(2)	0.0335	139.157	11.955	11

Ni-N(1.9) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	7(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	1(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(4)	1(3)	neg6(2)	0.0357	148.091	12.723	11

Ni-N(1.9) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(4)	9(4)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.86(3)	9(4)					
0.7Imd	1.99(3)	2(3)	neg6(2)	0.0349	144.789	12.439	11

Ni-N(1.9) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(5)	12(6)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.86(3)	8(4)					
1Imd	1.99(3)	3(3)	neg5(2)	0.0345	143.189	12.302	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	7(3)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.88(3)	9(4)					
0.5Imd	2.00(4)	1(3)	neg5(2)	0.0335	139.104	11.951	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	8(3)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)	neg5(1)	0.0326	135.172	11.613	11

4C	2.88(3)	9(4)					
0.7Imd	2.00(3)	2(3)					

Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	11(5)					
1S	2.36(1)	1(1)					
1S	2.21(1)	1(0)					
4C	2.87(3)	9(4)					
1Imd	1.99(3)	3(3)	neg4(1)	0.0321	133.421	11.463	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	8(3)					
1S	2.36(1)	1(1)					
1S	2.21(8)	2(0)					
4C	2.88(3)	9(4)					
0.7Imd	2.00(3)	2(3)	neg5(1)	0.0322	133.835	11.498	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	7(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(3)	1(3)	neg5(1)	0.034	141.22	12.133	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	8(4)					
1S	2.36(1)	1(1)					
1S	2.21(1)	2(0)					
4C	2.87(3)	9(4)					
0.7Imd	1.99(4)	2(3)	neg5(2)	0.0341	141.772	12.18	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	10(5)					
1S	2.36(1)	1(1)					
1S	2.21(1)	1(0)					
4C	2.86(3)	9(4)					
1Imd	1.99(3)	3(3)	neg5(2)	0.0334	138.87	11.931	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	8(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(3)	1(3)	neg5(1)	0.0342	142.193	12.216	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(4)	10(4)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.7Imd	1.99(3)	2(3)	neg5(1)	0.0338	140.535	12.074	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(4)	10(5)					
1S	2.36(1)	1(1)					
1S	2.21(1)	1(0)					
4C	2.87(3)	9(4)					
1Imd	1.99(3)	3(3)	neg5(2)	0.0339	140.954	12.11	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.4) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	8(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	1(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(4)	1(3)	neg5(2)	0.0347	144.157	12.385	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.4) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	9(4)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.7Imd	1.99(3)	2(3)	neg5(2)	0.034	141.366	12.145	11

Ni-N(2.0) Ni-S(2.1) Ni-S(2.4) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(5)	13(6)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)	neg5(2)	0.0338	140.244	12.049	11

4C	2.86(3)	8(4)					
1Imd	1.99(3)	3(3)					

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.97(3)	8(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(4)	1(3)	neg6(2)	0.0348	144.72	12.433	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	10(4)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.7Imd	1.99(3)	2(3)	neg5(2)	0.0342	142.16	12.213	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(6)	14(7)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.86(3)	8(3)					
1Imd	1.98(3)	3(3)	neg5(2)	0.034	141.05	12.118	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	8(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	1(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(4)	1(3)	neg6(2)	0.036	149.513	12.845	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	10(4)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.86(3)	9(4)					
0.7Imd	1.98(3)	2(3)	neg6(2)	0.0352	146.22	12.562	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(6)	13(7)	neg6(2)	0.0348	144.43	12.408	11

1S	2.20(1)	1(1)					
1S	2.36(1)	2(1)					
4C	2.86(3)	8(4)					
1Imd	1.98(3)	3(3)					

Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	6(1)					
1S	2.10(2)	4(2)					
1S	2.29(2)	1(2)					
4C	2.90(4)	10(6)					
0.5Imd	2.00(4)	0(3)	neg3(2)	0.0489	202.956	17.437	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	3(2)					
1S	2.30(2)	2(2)					
4C	2.90(4)	10(5)					
0.7Imd	2.00(3)	1(3)	neg3(2)	0.0414	171.793	14.759	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	3(2)					
1S	2.30(2)	2(2)					
4C	2.89(3)	10(5)					
1Imd	2.00(3)	2(2)	neg3(2)	0.0335	139.118	11.952	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	6(1)					
1S	2.10(2)	4(2)					
1S	2.29(2)	1(2)					
4C	2.90(4)	10(6)					
0.5Imd	2.00(4)	0(3)	neg3(2)	0.0491	204.035	17.529	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	3(2)					
1S	2.30(2)	2(2)					
4C	2.89(4)	10(5)					
0.7Imd	2.00(3)	1(3)	neg3(2)	0.0415	172.435	14.814	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	2(2)					
1S	2.31(2)	2(2)					
4C	2.89(3)	10(5)					
1Imd	2.00(3)	2(2)	neg3(2)	0.0336	139.433	11.979	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	5(1)					
1S	2.10(2)	4(2)					
1S	2.30(2)	2(2)					
4C	2.89(4)	10(6)					
0.5Imd	1.99(4)	0(3)	neg3(2)	0.0496	206.064	17.704	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	3(2)					
1S	2.30(2)	2(2)					
4C	2.89(4)	10(5)					
0.7Imd	2.00(3)	1(3)	neg3(2)	0.0419	173.891	14.94	11

Ni-N(2.1) Ni-S(2.1) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	2(2)					
1S	2.31(2)	3(2)					
4C	2.88(3)	9(4)					
1Imd	2.00(3)	2(2)	neg3(2)	0.0338	140.358	12.059	11

Ni-N(2.1) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	8(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(4)	1(3)	neg6(2)	0.0355	147.226	12.649	11

Ni-N(2.1) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	3(2)					
1S	2.30(2)	2(2)	neg3(2)	0.0489	203.156	17.454	11

4C	2.89(4)	9(5)					
0.7Imd	2.00(3)	0(2)					

Ni-N(2.1) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	5(1)					
1S	2.11(2)	2(2)					
1S	2.30(2)	2(2)					
4C	2.89(3)	9(4)					
1Imd	2.00(2)	2(2)	neg3(2)	0.0392	162.846	13.991	11

Ni-N(2.1) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(3)	8(3)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.99(3)	1(3)	neg6(2)	0.0357	148.048	12.719	11

Ni-N(2.1) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.99(4)	10(5)					
1S	2.20(1)	1(0)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.7Imd	1.98(3)	2(3)	neg6(2)	0.035	145.335	12.486	11

Ni-N(2.1) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(6)	15(7)					
1S	2.20(1)	1(1)					
1S	2.36(1)	2(1)					
4C	2.86(3)	8(4)					
1Imd	1.98(3)	3(2)	neg5(2)	0.0346	143.557	12.333	11

Ni-N(2.1) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.98(4)	8(4)					
1S	2.20(1)	1(1)					
1S	2.36(1)	2(1)					
4C	2.87(3)	9(4)					
0.5Imd	1.98(4)	1(3)	neg6(2)	0.0366	152.193	13.075	11

Ni-N(2.1) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	5(2)					
1S	2.11(2)	3(2)					
1S	2.30(2)	2(2)					
4C	2.89(4)	9(5)					
0.7Imd	2.00(3)	0(2)	neg3(2)	0.0565	234.806	20.173	11

Ni-N(2.1) Ni-S(2.3) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	4(1)					
1S	2.12(2)	2(3)					
1S	2.31(2)	3(2)					
4C	2.88(4)	9(4)					
1Imd	2.00(2)	1(2)	neg3(2)	0.0447	185.63	15.948	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(7)	15(8)					
1S	2.20(1)	1(1)					
1S	2.36(2)	2(1)					
2C	2.84(3)	3(3)					
1Imd	1.97(2)	2(2)	neg6(2)	0.0404	167.861	14.421	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(7)	15(8)					
1S	2.20(1)	1(1)					
1S	2.36(2)	2(1)					
2C	2.84(3)	3(3)					
1Imd	1.97(2)	2(2)	neg6(2)	0.0401	166.315	14.289	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(6)	10(10)					
1S	2.20(1)	1(1)					
1S	3.37(2)	3(2)					
1C	2.81(3)	1(3)					
1C	2.95(7)	1(9)					
1Imd	1.97(5)	4(6)	neg5(2)	0.0369	153.032	15.875	13

Ni-N(1.9) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(6)	4(8)	neg6(2)	0.0405	168.318	17.461	13

1S	2.20(1)	1(1)					
1S	3.36(2)	2(2)					
1C	2.80(4)	1(6)					
1C	2.92(9)	1(14)					
1Imd	1.97(6)	4(7)					

Ni-N(2.1) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	4(1)					
1S	2.25(3)	2(4)					
1S	2.41(5)	8(7)					
1C	2.85(3)	3(2)					
1C	3.06(3)	3(3)					
1Imd	1.94(2)	2(2)	neg3(2)	0.0379	157.416	16.33	13

Ni-N(1.9) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(6)	10(10)					
1S	2.20(1)	1(1)					
1S	2.37(2)	3(2)					
1C	2.81(3)	1(4)					
1C	2.95(8)	1(10)					
1Imd	1.97(5)	5(7)	neg5(2)	0.0376	156.178	16.202	13

Ni-N(2.1) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	2(1)					
1S	2.21(7)	9(15)					
1S	2.38(5)	10(15)					
1C	2.84(3)	2(2)					
1C	3.05(4)	2(3)					
1Imd	1.94(2)	1(2)	neg2(2)	0.0348	144.374	14.977	13

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.9) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(6)	10(9)					
1S	2.20(1)	1(1)					
1S	2.36(2)	2(2)					
1C	2.81(3)	1(4)					
1C	2.95(8)	1(10)					
1Imd	1.97(5)	4(6)	neg4(2)	0.0371	154.218	15.998	13

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.03(6)	10(10)					
1S	2.20(1)	1(1)					
1S	2.37(2)	3(2)					
1C	2.81(3)	1(4)					
1C	2.95(8)	1(10)					
1Imd	1.97(5)	4(6)	neg5(2)	0.0372	154.477	16.025	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	2(1)					
1N/O	2.08(1)	5(1)					
1S	2.31(3)	6(3)					
1S	2.55(7)	16(10)					
2C	2.93(5)	5(5)					
1Imd	2.04(3)	3(3)	0(2)	0.0226	93.668	9.717	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	3(1)					
1N/O	2.08(1)	5(1)					
1S	2.28(3)	5(4)					
1S	2.46(0.11)	18(14)					
3C	2.93(4)	7(4)					
0.5Imd	2.04(3)	0(3)	neg1(2)	0.0247	102.753	10.659	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(1)					
1N/O	2.08(1)	5(1)					
1S	2.27(5)	7(5)					
1S	2.41(0.15)	20(22)					
4C	2.93(4)	10(4)					
0.5Imd	2.03(3)	0(3)	neg2(2)	0.0242	100.609	10.437	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	3(1)					
1N/O	2.08(1)	5(1)					
1S	2.28(4)	6(4)					
1S	2.45(0.11)	18(15)					
3C	2.93(4)	7(4)					
0.5Imd	2.04(3)	0(3)	neg1(2)	0.0248	103.141	10.7	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(1)					
1N/O	2.08(1)	5(1)					
1S	2.27(5)	7(5)					
1S	2.40(0.14)	19(22)					
4C	2.93(4)	10(4)					
0.5Imd	2.03(3)	0(3)	neg2(2)	0.0243	101.016	10.479	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(0.21)	13(25)					
1N/O	1.97(8)	3(6)					
1S	2.35(2)	1(1)					
1S	2.21(1)	2(1)					
3C	2.87(4)	7(5)					
0.5Imd	2.00(4)	0(4)	neg5(2)	0.0373	155.07	16.087	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(0.20)	15(24)					
1N/O	1.96(5)	2(4)					
1S	2.35(2)	1(1)					
1S	2.21(1)	2(1)					
4C	2.88(4)	9(4)					
0.5Imd	2.00(4)	1(4)	neg5(2)	0.033	137.172	14.23	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	1(2)					
1N/O	2.08(1)	4(1)					
1S	2.38(6)	8(10)					
1S	2.23(5)	5(6)					
4C	2.92(4)	9(4)					
0.7Imd	2.03(4)	2(3)	neg2(2)	0.0276	114.569	11.885	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	1(2)					
1N/O	2.07(1)	4(1)					
1S	2.38(5)	7(8)					
1S	2.23(4)	4(6)					
4C	2.92(4)	9(4)					
0.7Imd	2.03(3)	1(3)	neg2(2)	0.027	111.944	11.613	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(2)					
1N/O	2.08(1)	4(1)					
1S	2.39(0.20)	22(35)					
1S	2.27(6)	9(6)					
4C	2.93(4)	10(5)					
1Imd	2.04(4)	4(4)	neg1(2)	0.0263	109.343	11.343	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	2(2)					
1N/O	2.07(1)	4(1)					
1S	2.39(6)	8(10)					
1S	2.24(5)	5(6)					
4C	2.92(4)	9(4)					
0.7Imd	2.03(4)	2(3)	neg2(2)	0.028	116.084	12.042	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	2(2)					
1N/O	2.08(1)	4(1)					
1S	2.26(6)	7(6)					
1S	2.39(0.11)	16(20)					
4C	2.93(4)	10(5)					
0.7Imd	2.03(4)	2(4)	neg2(2)	0.028	116.086	12.043	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(0.20)	13(24)					
1N/O	1.97(7)	3(6)					
1S	2.35(2)	1(1)					
1S	2.21(1)	2(1)					
3C	2.87(4)	7(5)					
0.5Imd	2.00(4)	1(4)	neg5(2)	0.0368	152.999	15.872	13

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(0.19)	15(24)					
1N/O	1.96(5)	2(4)					
1S	2.35(2)	1(1)					
1S	2.20(1)	2(1)	neg5(2)	0.0326	135.274	14.033	13

4C	2.88(4)	10(4)					
0.5Imd	2.00(4)	1(4)					

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(1)					
1N/O	2.08(1)	5(1)					
1S	2.28(4)	7(4)					
1S	2.42(0.21)	26(29)					
4C	2.94(5)	12(6)					
0.7Imd	2.02(4)	3(4)	neg1(2)	0.0234	96.986	10.061	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(1)					
1N/O	2.08(1)	5(1)					
1S	2.28(4)	7(4)					
1S	2.44(0.20)	27(29)					
4C	2.94(5)	12(6)					
0.7Imd	2.02(4)	3(4)	neg1(2)	0.0234	97.206	10.084	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(0.35)	27(44)					
1N/O	1.96(4)	3(4)					
1S	2.20(1)	2(1)					
1S	2.35(2)	1(1)					
4C	2.86(4)	9(4)					
0.7Imd	1.99(4)	2(4)	neg6(2)	0.0327	135.969	14.105	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	3(1)					
1N/O	2.08(1)	5(1)					
1S	2.28(4)	6(4)					
1S	2.44(0.12)	18(16)					
3C	2.93(4)	7(4)					
0.5Imd	2.04(3)	0(3)	neg1(2)	0.0247	102.643	10.648	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(2)					
1N/O	2.08(1)	5(1)	neg2(2)	0.0242	100.499	10.426	13

1S	2.27(5)	7(5)					
1S	2.38(0.16)	20(25)					
4C	2.93(4)	10(4)					
0.5Imd	2.03(3)	0(3)					

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(2)					
1N/O	2.08(1)	5(1)					
1S	2.28(3)	7(4)					
1S	2.43(0.23)	27(32)					
4C	2.93(5)	12(6)					
0.7Imd	2.02(4)	3(4)	neg1(2)	0.0235	97.718	10.137	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O							
1N/O							
1S							
1S							
4C							
0.7Imd			No Fit	No Fit	No Fit	No Fit	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-C(2.8) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(1)					
1N/O	2.08(1)	5(1)					
1S	2.29(3)	7(4)					
1S	2.46(0.18)	25(27)					
4C	2.93(5)	12(6)					
0.7Imd	2.02(4)	3(4)	neg1(2)	0.0235	97.426	10.107	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(2)	3(1)					
1N/O	2.08(1)	5(1)					
1S	2.43(0.10)	14(14)					
1S	2.28(4)	5(4)					
3C	2.93(4)	7(4)					
0.5Imd	2.04(3)	0(3)	neg1(2)	0.0249	103.557	10.743	13

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.95(2)	2(2)					
1N/O	2.08(1)	5(1)					
1S	2.38(0.13)	16(23)					
1S	2.26(6)	7(6)					
4C	2.93(4)	10(4)					
0.5Imd	2.03(3)	0(3)	neg1(2)	0.0242	100.582	10.434	13

Ni-N(1.8) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.1) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(0.25)	16(46)					
1N/O	2.03(0.18)	5(15)					
1S	2.20(2)	1(1)					
1S	2.36(3)	2(2)					
1C	2.81(4)	1(5)					
1C	2.94(0.10)	2(15)					
1Imd	1.97(6)	4(7)	neg5(3)	0.037	153.691	20.118	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.1) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	1(3)					
1N/O	2.08(1)	4(1)					
1S	2.27(0.10)	9(7)					
1S	2.37(0.16)	21(38)					
2C	2.86(3)	2(3)					
2C	3.03(6)	4(6)					
1Imd	1.99(4)	4(5)	neg2(2)	0.0189	78.645	10.294	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.1) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	2(2)					
1N/O	2.08(1)	5(1)					
1S	2.29(3)	4(3)					
1S	2.50(7)	12(8)					
1C	2.88(3)	2(3)					
1C	3.03(4)	1(4)					
1Imd	2.01(5)	5(6)	0(2)	0.0183	75.849	9.928	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	2(2)					
1N/O	2.08(1)	5(1)					
1S	2.29(3)	4(3)					
1S	2.50(7)	12(7)					
1C	2.88(3)	2(3)	0(2)	0.0182	75.668	9.905	15

1C	3.03(4)	1(4)
1Imd	2.01(5)	5(6)

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.1) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	1(2)					
1N/O	2.08(1)	5(1)					
1S	2.28(4)	6(4)					
1S	2.46(0.11)	18(15)					
2C	2.89(3)	2(3)					
1C	3.06(5)	0(3)					
1Imd	2.00(5)	4(6)	neg1(2)	0.0183	76.176	9.971	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.1) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(2)	1(2)					
1N/O	2.08(1)	5(1)					
1S	2.28(4)	6(4)					
1S	2.46(0.10)	15(12)					
1C	2.85(3)	1(3)					
2C	3.01(5)	4(7)					
1Imd	2.00(4)	4(6)	neg1(2)	0.0184	76.417	10.003	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-C(2.9) Ni-C(3.1) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(2)	1(3)					
1N/O	2.08(1)	4(1)					
1S	2.27(9)	9(7)					
1S	2.38(0.15)	21(36)					
1C	2.86(3)	2(3)					
2C	3.03(6)	4(6)					
1Imd	1.99(4)	4(5)	neg2(2)	0.0189	78.629	10.292	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(0.22)	14(26)					
1N/O	1.96(6)	2(5)					
1S	2.35(2)	1(1)					
1S	2.21(1)	2(1)					
4C	2.88(4)	10(5)					
1Cl	3.56(0.15)	18(23)					
0.5Imd	2.01(5)	1(4)	neg5(2)	0.0331	137.602	18.012	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	1(2)					
1N/O	2.07(2)	4(1)					
1S	2.38(5)	7(9)					
1S	2.23(5)	4(7)					
4C	2.91(4)	9(4)					
1Cl	3.40(0.50)	45(103)					
0.7Imd	2.03(4)	1(3)	neg2(2)	0.0265	109.995	14.398	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	1(2)					
1N/O	2.08(1)	4(1)					
1S	2.33(0.29)	21(50)					
1S	2.27(0.12)	10(12)					
4C	2.91(6)	9(5)					
1Cl	3.34(0.51)	45(109)					
1Imd	2.03(5)	3(4)	neg2(3)	0.0262	108.931	14.259	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(0.22)	14(26)					
1N/O	1.96(6)	2(5)					
1S	2.35(2)	1(1)					
1S	2.21(1)	2(1)					
4C	2.88(4)	10(5)					
1Cl	3.56(0.15)	18(23)					
0.5Imd	2.01(5)	1(4)	neg5(2)	0.0331	137.61	18.013	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(3)	1(2)					
1N/O	2.07(2)	4(1)					
1S	2.38(5)	7(9)					
1S	2.23(5)	4(7)					
4C	2.91(4)	9(4)					
1Cl	2.40(0.50)	45(103)					
0.7Imd	2.03(4)	1(3)	neg2(2)	0.0265	109.941	14.391	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(3)	1(2)					
1N/O	2.08(1)	4(1)					
1S	2.36(9)	10(24)	neg2(2)	0.0262	108.957	14.262	15

1S	2.23(0.12)	8(16)
4C	2.91(5)	9(5)
1Cl	3.33(0.45)	42(93)
1Imd	2.03(5)	3(4)

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.92(0.17)	15(24)					
1N/O	1.95(4)	1(3)					
1S	2.35(2)	1(1)					
1S	2.20(1)	2(1)					
4C	2.87(4)	9(5)					
1Cl	4.01(7)	8(8)					
0.5Imd	2.02(5)	1(4)	neg6(2)	0.0286	118.625	15.528	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(2)	2(2)					
1N/O	2.07(2)	4(2)					
1S	2.37(5)	7(9)					
1S	2.22(5)	4(7)					
4C	2.92(4)	8(4)					
1Cl	4.01(4)	5(5)					
0.7Imd	2.05(4)	1(3)	neg2(2)	0.025	104.002	13.613	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	4(2)					
1N/O	1.93(2)	2(2)					
1S	2.37(5)	7(11)					
1S	2.22(6)	5(9)					
4C	2.91(4)	7(3)					
1Cl	4.00(4)	5(5)					
1Imd	2.05(3)	1(3)	neg3(2)	0.0285	118.25	15.478	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.92(0.17)	15(24)					
1N/O	1.95(4)	1(3)					
1S	2.35(2)	1(1)					
1S	2.20(1)	2(1)					
4C	2.88(4)	9(4)					
1Cl	4.01(6)	7(8)					
0.5Imd	2.02(5)	1(4)	neg6(2)	0.0285	118.45	15.505	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.94(4)	1(3)					
1N/O	1.92(0.18)	17(29)					
1S	2.35(2)	1(1)					
1S	2.20(1)	2(1)					
4C	2.88(4)	9(4)					
1Cl	4.00(6)	6(7)					
0.7Imd	2.02(4)	1(4)	neg5(2)	0.0272	112.954	14.785	15

Ni-N(1.8) Ni-N(1.9) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	4(2)					
1N/O	1.93(2)	2(2)					
1S	2.37(5)	7(11)					
1S	2.22(6)	5(9)					
4C	2.91(4)	7(3)					
1Cl	4.00(4)	4(4)					
1Imd	2.05(3)	1(3)	neg2(2)	0.0282	117.31	15.355	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(3.9) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(2)					
1N/O	2.08(1)	5(1)					
1S	2.26(8)	8(6)					
1S	2.36(0.16)	19(29)					
4C	2.92(4)	10(5)					
1Cl	4.17(0.19)	20(30)					
0.5Imd	2.03	0(3)	neg2(2)	0.0219	90.89	11.897	15

Ni-N(1.9) Ni-N(2.0) Ni-S(2.1) Ni-S(2.2) Ni-C(2.9) Ni-Cl(4.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(2)	2(2)					
1N/O	2.08(1)	5(1)					
1S	2.26(7)	8(6)					
1S	2.36(0.16)	19(29)					
4C	2.92(4)	10(5)					
1Cl	4.17(0.19)	19(30)					
0.5Imd	2.03(4)	0(3)	neg2(2)	0.0219	90.944	11.904	15

APPENDIX J

ADDITIONAL FIT TABLES FOR INRS

Table J.1. Additional Fits for Ni(II) WT-InrS in Buffer with 10 mM Hepes, 1 M NaBr, 5 mM TCEP at pH 8.1.

Data Fit from k = 2 - 14 Å^{-1} and r = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(2)	1(1)	14(3)	0.3839	3632.787	184.972	3
3N/O	2.09(2)	3(1)	12(2)	0.3919	3265.393	166.265	3
4N/O	2.08(2)	7(2)	10(2)	0.4378	3647.894	185.741	3
5N/O	2.05(3)	10(3)	7(3)	0.4812	4009.593	204.158	3
6N/O	2.04(3)	13(4)	6(3)	0.5209	4340.373	221.001	3
7N/O	2.03(4)	16(4)	4(3)	0.5605	4669.883	237.778	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.22(1)	5(1)	0(3)	0.2126	1771.252	90.188	3
3S	2.21(2)	8(1)	neg1(3)	0.2018	1681.180	85.601	3
4S	2.21(2)	11(1)	neg3(3)	0.2255	1879.125	95.680	3
5S	2.20(2)	14(2)	neg4(3)	0.2602	2167.919	110.385	3
6S	2.19(2)	16(2)	neg5(3)	0.2973	2477.274	126.136	3
7S	2.19(3)	18(2)	neg6(3)	0.3338	2781.375	141.620	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.09(2)	1(1)					
1N/O	1.94(3)	0(2)	8(2)	0.2913	2427.170	137.597	5
2N/O	1.95(3)	4(3)					
2N/O	2.10(1)	1(1)	6(2)	0.2873	2393.776	135.704	5
3N/O	2.08(2)	1(1)					
1N/O	1.91(2)	1(2)	7(2)	0.2844	2369.166	134.309	5
4N/O	2.09(2)	6(2)					
1N/O	1.46(0.11)	37(38)	13(3)	0.3928	3272.723	185.532	5
3N/O	2.08(2)	1(1)					
2N/O	1.92(2)	3(2)	5(2)	0.3042	2534.865	143.703	5
5N/O	2.06(3)	10(3)					
1N/O	1.52(0.19)	37(49)	10(4)	0.4529	3773.601	213.927	5

4N/O	2.11(2)	6(2)					
2N/O	1.49(7)	52(28)	16(3)	0.3544	2952.416	167.374	5
3N/O	2.09(2)	1(1)					
3N/O	1.92(3)	6(3)	4(2)	0.3473	2893.803	164.051	5
6N/O	2.04(4)	13(4)					
1N/O	3.34(9)	1(8)	5(3)	0.5094	4244.071	240.598	5
5N/O	2.06(2)	10(2)					
2N/O	2.51(3)	4(4)	8(2)	0.2836	2362.811	133.949	5
4N/O	2.12(2)	6(2)					
3N/O	1.52(5)	61(21)	18(3)	0.3201	2667.250	151.208	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.20(1)	3(1)					
1S	2.05(2)	5(2)	neg8(3)	0.1498	1247.983	70.749	5
2S	2.20(1)	3(1)					
2S	2.06(2)	9(2)	neg10(2)	0.1354	1128.024	63.948	5
3S	2.18(1)	5(1)					
1S	2.00(2)	4(1)	neg9(2)	0.1276	1062.869	60.255	5
4S	2.21(2)	11(1)					
1S	2.61(4)	8(5)	neg3(3)	0.1697	1413.792	80.149	5
3S	2.19(1)	5(1)					
2S	2.02(2)	8(2)	neg11(2)	0.1367	1138.859	64.562	5
5S	2.20(2)	14(2)					
1S	2.51(0.13)	11(17)	neg4(3)	0.2521	2100.548	119.081	5
4S	2.22(2)	11(1)					
2S	1.72(0.10)	51(31)	1(4)	0.2098	1748.401	99.118	5
3S	2.19(1)	5(1)					
3S	2.03(2)	11(2)	neg12(2)	0.1559	1298.940	73.638	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.21(3)	14(2)					
2S	1.78(0.16)	52(37)	neg2(4)	0.2452	2042.648	115.799	5
4S	2.19(1)	7(1)					
3S	2.01(2)	11(2)	neg12(2)	0.1837	1530.922	86.789	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.95(4)	8(3)					5
1S	2.22(1)	1(1)	0(3)	0.1627	1355.821	76.862	
1N/O	1.87(2)	2(2)					5
2S	2.20(1)	4(1)	neg3(2)	0.1230	1025.041	58.110	
2N/O	1.89(3)	7(3)					
2S	2.21(1)	4(1)	neg3(2)	0.1428	1189.994	67.461	5
3N/O	1.97(5)	12(4)					
1S	2.22(1)	2(1)	1(3)	0.1593	1326.961	75.226	5
1N/O	2.06(0.26)	29(82)					
3S	2.22(2)	8(1)	0(4)	0.1934	1611.220	91.341	5
1N/O	1.28(0.15)	28(40)					
4S	2.21(2)	11(1)	neg1(3)	0.2156	1796.253	101.830	5
4N/O	1.99(6)	17(5)					
1S	2.22(1)	2(1)	2(4)	0.1685	1403.890	79.587	5
2N/O	2.14(0.12)	30(80)					
3S	2.22(2)	8(2)	2(7)	0.1855	1545.713	87.627	5
3N/O	2.07(0.12)	25(18)					
2S	2.23(2)	6(1)	4(6)	0.1632	1359.670	77.080	5
5N/O	2.01(8)	22(5)					
1S	2.22(1)	2(1)	2(5)	0.1815	1511.906	85.711	5
1N/O	2.36(3)	0(2)					
5S	2.21(3)	15(2)	neg5(4)	0.2097	1746.746	99.024	5
4N/O	2.11(0.10)	30(21)					
2S	2.23(2)	5(1)	5(5)	0.1602	1334.551	75.656	5
2N/O	2.11(1)	1(1)					
4S	2.16(2)	11(2)	neg3(3)	0.1436	1196.634	67.838	5
3N/O	2.17(7)	25(37)					
3S	2.23(2)	8(1)	4(6)	0.1761	1467.213	83.177	5
6N/O	2.02(0.10)	27(6)					
1S	2.22(2)	2(1)	3(5)	0.1946	1621.068	91.899	5
1N/O	2.36(2)	1(2)	neg6(4)	0.2260	1882.639	106.728	5

6S	2.20(3)	17(2)					
5N/O	2.13(9)	35(20)					
2S	2.23(2)	5(1)	5(5)	0.1585	1320.340	74.851	5
2N/O	1.32(0.17)	53(53)					
5S	2.21(2)	14(2)	neg2(3)	0.2523	2102.244	119.177	5
4N/O	2.19(5)	26(20)					
3S	2.24(1)	8(1)	6(4)	0.1670	1391.411	78.880	5
3N/O	2.12(2)	2(1)					
4S	2.17(2)	11(3)	1(3)	0.1456	1212.783	68.753	5

Ni-N(2.0) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.84(4)	5(3)					5
1Br	2.27(2)	5(1)	neg2(7)	0.3501	2916.769	165.353	
1N/O	1.82(2)	1(2)					5
2Br	2.27(2)	8(1)	neg23(6)	0.2686	2238.185	126.884	
2N/O	1.83(3)	5(2)					
2Br	2.27(2)	8(10)	neg22(6)	0.2541	2116.858	120.006	5
3N/O	2.08(2)	5(2)					
1Br	2.43(3)	10(3)	10(2)	0.2873	2393.329	135.679	5
1N/O	1.82(2)	1(2)					
3Br	2.27(2)	10(1)	neg23(5)	0.2158	1798.130	101.937	5
1N/O	1.82(2)	1(1)					
4Br	2.27(2)	12(1)	neg23(4)	0.1864	1553.433	88.065	5
4N/O	2.04(3)	10(3)					
1Br	2.40(3)	9(3)	6(3)	0.3040	2533.085	143.602	5
2N/O	1.82(2)	5(2)					
3Br	2.28(2)	10(1)	neg22(5)	0.2096	1746.043	98.984	5
3N/O	1.83(3)	8(3)					
2Br	2.28(2)	8(1)	neg21(6)	0.2534	2111.202	119.685	5
5N/O	2.02(4)	13(4)					
1Br	2.38(2)	8(2)	4(3)	0.3155	2628.759	149.026	5
1N/O	1.81(2)	1(1)					
5Br	2.28(2)	13(1)	neg23(4)	0.1697	1414.208	80.172	5

4N/O	1.84(4)	11(4)					
2Br	2.28(2)	8(1)	neg20(6)	0.2556	2129.651	120.731	5
2N/O	1.82(2)	5(2)					
4Br	2.28(2)	12(1)	neg22(4)	0.1869	1557.192	88.278	5
3N/O	1.83(3)	8(3)					
3Br	2.28(2)	10(1)	neg21(5)	0.2147	1788.820	101.409	5
6N/O	2.00(5)	17(4)					
1Br	2.36(2)	8(2)	1(4)	0.3306	2754.803	156.171	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.01(4)	15(4)					
2Br	2.39(2)	11(2)	3(3)	0.2682	2234.156	126.655	5
2N/O	1.81(2)	5(2)					
5Br	2.28(2)	13(1)	neg22(4)	0.1757	1463.729	82.979	5
4N/O	1.83(4)	12(4)					
3Br	2.29(2)	10(1)	neg20(6)	0.2199	1832.112	103.863	5
3N/O	1.82(3)	8(3)					
4Br	2.28(2)	12(1)	neg21(5)	0.1959	1632.401	92.542	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.01(3)	14(4)					
1Imd	2.09(2)	1(1)	6(2)	0.3407	3223.784	182.758	5
4N/O	2.01(5)	16(8)					
1Imd	1.96(6)	3(7)					
1Imd	2.09(2)	2(2)	6(2)	0.2918	2430.980	155.437	7
3N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	2346.537	172.038	9
2N/O	2.04(5)	8(7)					
1Imd	2.01(4)	6(3)					
1Imd	2.13(3)	5(3)					
1Imd	1.88(4)	3(3)					
1Imd	1.60(7)	13(11)	8(2)	0.1876	1563.006	134.283	11
1N/O	2.08(4)	0(4)					
1Imd	2.04(4)	11(5)	7(3)	0.1801	1500.320	155.641	13

1Imd	1.94(4)	11(5)					
1Imd	2.15(4)	9(5)					
1Imd	1.63(9)	11(13)					
1Imd	1.83(4)	7(5)					
4N/O	2.02(3)	11(4)					
1Imd	2.10(2)	1(1)	8(2)	0.3117	2596.635	147.204	5
3N/O	2.04(4)	10(6)					
1Imd	1.94(6)	3(5)					
1Imd	2.09(2)	2(1)	7(2)	0.2670	2224.612	142.242	7
2N/O	2.04(5)	8(8)					
1Imd	1.89(3)	3(3)					
1Imd	2.01(3)	6(3)					
1Imd	2.13(3)	6(3)	7(2)	0.2305	1920.469	140.800	9
1N/O	2.09(3)	0(3)					
1Imd	2.00(3)	7(3)					
1Imd	1.60(8)	17(15)					
1Imd	1.88(3)	4(3)					
1Imd	2.12(3)	6(3)	8(2)	0.1887	1572.161	135.069	11
0N/O							
1Imd	2.06(3)	13(3)					
1Imd	1.85(3)	8(3)					
1Imd	1.95(3)	12(3)					
1Imd	1.64(0.14)	19(22)					
1Imd	2.16(2)	11(3)	7(3)	0.2256	1879.542	161.478	11
3N/O	2.03(3)	8(4)					
1Imd	2.11(2)	1(1)	12(2)	0.2804	2336.347	132.449	5
2N/O	2.08(3)	3(3)					
1Imd	2.09(3)	1(2)					
1Imd	1.93(3)	0(1)	10(2)	0.2476	2062.537	131.879	7
1N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
1Imd	1.96(2)	12(3)					
1Imd	2.06(2)	13(3)					
1Imd	1.86(3)	7(2)					
1Imd	2.17(2)	10(3)	7(2)	0.2519	2099.118	153.898	9
2N/O	2.05(4)	6(4)					
1Imd	2.11(2)	1(1)	12(2)	0.3051	2542.292	144.124	5

1N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7
0N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(8)	13(9)					
1S	2.22(1)	1(1)					
1Imd	1.95(6)	7(8)	0(3)	0.1291	1075.218	68.749	7
1N/O	1.97(9)	13(13)					
1S	2.24(1)	2(1)					
1Imd	1.89(2)	0(2)					
1Imd	2.03(2)	2(1)	3(2)	0.0692	576.201	42.245	9
1S	2.24(1)	3(1)					
1Imd	1.99(2)	5(2)					
1Imd	1.87(2)	4(1)					
1Imd	2.11(2)	3(3)	4(1)	0.0646	537.905	39.437	9

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.96(8)	13(9)					
1S	2.22(1)	1(1)					
1Imd	1.95(6)	7(7)	0(3)	0.1284	1070.093	68.422	7
1N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1S	2.24(1)	2(1)					
1Imd	1.99(2)	5(2)					
1Imd	2.11(2)	3(3)					
1Imd	1.87(2)	4(1)	4(1)	0.0638	531.713	38.983	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.93(3)	6(3)					
1S	2.25(2)	2(1)					
1Imd	2.06(3)	0(2)	5(3)	0.1204	1003.298	64.151	7

1N/O	1.99(8)	10(11)					
1S	2.25(1)	2(1)					
1Imd	1.89(2)	0(1)					
1Imd	2.04(2)	2(1)	3(2)	0.0598	498.256	36.530	9
1S	2.24(1)	2(1)					
1Imd	2.10(2)	3(3)					
1Imd	1.87(2)	4(2)					
1Imd	1.99(2)	5(2)	4(1)	0.0634	528.250	38.729	9

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(3)	6(4)					
1S	2.72(3)	6(4)					
1Imd	2.11(2)	1(1)	11(2)	0.2425	2020.563	129.195	7
1N/O	2.09(3)	1(3)					
1S	2.72(5)	8(6)					
1Imd	1.94(3)	0(3)					
1Imd	2.09(3)	1(2)	9(2)	0.2280	1899.919	139.294	9
1S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(3)	6(4)					
1S	2.72(3)	6(4)					
1Imd	2.11(2)	1(1)	11(2)	0.2467	2055.517	131.430	7
1N/O	2.09(3)	1(3)					
1S	2.72(5)	8(6)					
1Imd	2.09(3)	1(2)					
1Imd	1.94(3)	0(3)	9(2)	0.2311	1925.478	141.168	9
1S	2.71(4)	6(5)					
1Imd	1.90(2)	5(2)					
1Imd	2.14(2)	7(2)					
1Imd	2.02(2)	8(2)	8(2)	0.2585	2153.940	157.918	9

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	6(3)					
1Br	2.43(2)	8(2)					
1Imd	2.10(1)	2(1)	9(2)	0.1678	1587.529	101.507	7
1N/O	2.07(2)	0(2)	7(2)	0.1151	959.281	70.330	9

1Br	2.42(2)	8(2)					
1Imd	1.92(2)	1(1)					
1Imd	2.07(2)	2(1)					

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.00(3)	6(3)					
1Br	2.43(2)	8(2)					
1Imd	2.10(1)	2(1)	9(2)	0.1714	1428.091	91.312	7
1N/O	2.07(2)	0(2)					
1Br	2.42(2)	8(2)					
1Imd	1.92(2)	1(1)					
1Imd	2.07(2)	2(1)	8(2)	0.1189	990.722	72.635	9

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(3)	6(3)					
1Br	2.43(2)	8(2)					
1Imd	2.10(1)	2(1)	9(2)	0.1714	1428.101	91.313	7
1N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	0(1)					
1Br	2.43(3)	9(3)					
1Imd	1.93(3)	2(3)	8(2)	0.2178	1814.333	116.009	7
1N/O	2.07(2)	0(2)					
1Br	2.42(2)	8(2)					
1Imd	2.07(2)	2(1)					
1Imd	1.92(2)	1(1)	8(2)	0.1242	1034.632	75.855	9

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(2)	2(2)					
2S	2.22(1)	5(1)					
1Imd	1.98(5)	5(4)	0(2)	0.0930	774.439	49.518	7
0N/O			2(1)	0.0490	408.669	26.130	9

2S	2.23(1)	5(1)					
1Imd	2.02(2)	1(1)					
1Imd	1.87(1)	1(1)					

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.81(0.27)	39(66)					
2S	2.20(1)	4(1)					
1Imd	1.87(2)	2(1)	neg5(2)	0.0940	782.911	50.059	7
0N/O							
2S	2.23(1)	6(1)					
1Imd	2.02(2)	0(1)					
1Imd	1.87(1)	1(1)	0(1)	0.0555	462.366	29.564	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.86(3)	3(3)					
2S	2.21(6)	6(6)					
1Imd	1.94(1)	5(1)	neg3(2)	0.1028	856.170	54.744	7
0N/O							
2S	2.23(1)	6(1)					
1Imd	2.01(2)	0(1)					
1Imd	1.87(1)	1(1)	neg1(1)	0.0564	469.762	30.037	9

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(5)	2(5)					
2S	2.76(5)	14(7)					
1Imd	2.12(3)	1(2)	14(2)	0.3576	2979.510	190.510	7
0N/O							
2S	3.06(0.21)	33(43)					
1Imd	2.00(4)	0(5)					
1Imd	2.11(2)	3(2)	12(3)	0.3727	3105.332	198.555	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(5)	2(6)					
2S	2.76(5)	13(7)					
1Imd	2.11(3)	1(2)	14(2)	0.3667	3055.150	195.346	7
0N/O			12(3)	0.3711	3091.789	197.689	9

2S	3.10(9)	17(15)					
1Imd	2.00(4)	0(5)					
1Imd	2.11(2)	3(2)					

Ni-N(2.0) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(5)	2(4)					
2Br	2.26(2)	8(1)					
1Imd	1.78(4)	1(2)	neg25(6)	0.2092	1742.973	111.446	7
0N/O							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(4)	4(5)					
2Br	2.44(2)	12(2)					
1Imd	2.10(2)	1(1)	10(2)	0.2008	1673.001	106.972	7
0N/O							
2Br	2.42(2)	11(2)					
1Imd	2.08(2)	3(1)					
1Imd	1.94(2)	1(2)	6(2)	0.1875	1773.831	113.419	9

Ni-N(2.0) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.10(1)	2(1)					
2Br	2.44(2)	13(2)					
1Imd	1.99(4)	3(4)	9(2)	0.2055	1712.091	109.471	7
0N/O							
2Br	2.42(2)	11(2)					
1Imd	2.08(2)	3(1)					
1Imd	1.94(2)	1(2)	7(2)	0.1927	1605.477	102.654	9

Ni-N(2.0) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.10(1)	2(1)					
2Br	2.44(2)	13(2)					
1Imd	1.99(4)	3(4)	9(2)	0.2097	1746.966	111.701	7
0N/O			12(2)	0.3357	2797.239	178.856	9

2Br	2.85(4)	13(4)					
1Imd	2.11(2)	2(2)					
1Imd	2.01(4)	1(5)					

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.76(0.21)	34(56)					
1S	2.14(3)	1(2)					
1S	2.25(2)	1(3)					
1Imd	1.86(2)	1(2)	neg5(3)	0.0926	771.106	56.534	9
1S	2.17(4)	8(7)					
1S	2.25(2)	2(2)					
1Imd	1.87(2)	1(1)					
1Imd	2.02(2)	1(1)	neg1(2)	0.0492	410.008	30.060	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.87(3)	2(2)					
1S	2.18(3)	1(2)					
1S	2.28(3)	2(3)					
1Imd	1.96(6)	6(7)	0(3)	0.0887	739.976	54.179	9
1S	2.18(4)	7(6)					
1S	2.26(3)	2(2)					
1Imd	2.02(2)	1(1)					
1Imd	1.87(1)	1(1)	0(2)	0.0425	353.819	25.940	9
1S	2.18(5)	7(7)					
1S	2.26(3)	3(2)					
1Imd							
0°	2.02(2)	1(1)					
1Imd							
5°	1.88(2)	1(1)	1(2)	0.0498	414.599	30.397	9
1S	2.19(0.21)	6(17)					
1S	2.24(0.17)	4(6)					
1Imd							
0°	1.86(2)	1(1)					
1Imd							
10°	2.01(4)	4(4)	neg1(3)	0.0816	680.185	49.868	9
1S	2.18(5)	10(8)					
1S	2.25(2)	2(1)					
1Imd							
5°	2.02(2)	2(1)					
1Imd							
5°	1.88(2)	1(1)	1(2)	0.0449	373.858	27.410	9

1S	2.19(0.17)	6(15)					
1S	2.23(0.12)	4(4)					
1Imd 5°	1.86(2)	1(1)					
1Imd 10°	2.01(3)	3(3)	neg1(3)	0.0819	682.618	50.047	9
1S							
1S							
1Imd 10°							
1Imd 10°			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(3)	4(4)					
1S	2.21(1)	1(1)					
1S	2.65(2)	4(2)					
1Imd	1.97(5)	5(4)	neg3(3)	0.0771	642.231	47.086	9
1S	2.24(1)	2(1)					
1S	2.68(3)	9(4)					
1Imd	1.88(2)	1(1)					
1Imd	2.02(2)	2(1)	1(2)	0.0657	547.133	40.113	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(3)	3(3)					
1S	2.21(1)	1(1)					
1S	2.65(2)	4(2)					
1Imd	1.97(5)	4(4)	neg2(3)	0.0779	648.835	47.570	9
1S	2.24(1)	2(1)					
1S	2.68(3)	9(4)					
1Imd	1.88(2)	1(1)					
1Imd	2.02(2)	2(1)	1(2)	0.0668	556.512	40.801	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.74(0.22)	36(60)					
1S	2.14(3)	1(2)					
1S	1.86(2)	1(2)					
1Imd	2.83(2)	1(3)	neg6(3)	0.0906	755.006	55.354	9
1S	2.25(2)	2(2)	neg1(2)	0.0489	407.719	29.892	9

1S	2.16(1)	1(1)					
1Imd	1.86(2)	1(1)					
1Imd	2.01(4)	7(7)					

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(4)	4(4)					
1S	2.21(1)	1(1)					
1S	2.64(2)	4(2)					
1Imd	1.95(6)	5(5)	neg3(3)	0.0763	635.344	46.581	9
1S	2.24(1)	2(1)					
1S	2.68(3)	9(4)					
1Imd	2.02(2)	2(1)					
1Imd	1.88(2)	1(1)	1(2)	0.0645	536.985	39.369	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(4)	4(4)					
1S	2.21(1)	1(1)					
1S	2.64(2)	4(2)					
1Imd	1.95(6)	5(5)	neg3(3)	0.0771	642.158	47.080	9
1S	2.24(1)	2(1)					
1S	2.68(3)	9(4)					
1Imd	2.02(2)	2(1)					
1Imd	1.88(2)	1(1)	1(2)	0.0655	545.823	40.017	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(4)	5(4)					
1S	2.64(1)	1(1)					
1S	2.20(6)	5(5)					
1Imd	1.94(2)	4(2)	neg4(3)	0.0718	598.191	43.857	9
1S	2.67(1)	2(1)					
1S	2.23(2)	1(1)					
1Imd	1.87(2)	2(1)					
1Imd	2.01(3)	8(4)	0(2)	0.0603	502.256	36.823	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(4)	5(4)					
1S	2.21(2)	4(2)	neg4(3)	0.0754	627.930	46.037	9

1S	2.64(6)	5(5)					
1Imd	1.95(1)	1(1)					
1S	2.23(1)	2(1)					
1S	2.67(3)	9(4)					
1Imd	2.01(2)	2(1)					
1Imd	1.87(2)	1(1)	0(2)	0.0640	533.598	39.121	9

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(5)	2(6)					
1S	2.76(5)	8(7)					
1S	3.10(5)	4(6)					
1Imd	2.12(3)	2(2)	14(3)	0.2660	2216.414	162.498	9
1S	2.75(6)	8(9)					
1S	3.06(5)	4(5)					
1Imd	2.11(2)	3(2)					
1Imd	2.01(4)	1(6)	12(3)	0.3128	2606.123	191.070	9

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(4)	4(5)					
1Br	2.36(2)	3(2)					
1Br	2.51(2)	4(2)					
1Imd	2.07(2)	1(2)	8(3)	0.1549	1290.385	94.605	9
0N/O							
1Br	2.33(2)	3(1)					
1Br	2.47(3)	4(2)					
1Imd	1.88(2)	1(2)					
1Imd	2.02(2)	3(1)	0(3)	0.1474	1228.214	90.047	9

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(4)	4(5)					
1Br	2.36(2)	3(2)					
1Br	2.51(2)	4(2)					
1Imd	2.07(2)	1(2)	8(3)	0.1575	1311.869	96.181	9
0N/O							
1Br	2.33(2)	3(1)					
1Br	2.47(3)	5(2)					
1Imd	2.02(2)	3(1)					
1Imd	1.88(2)	1(2)	0(3)	0.1499	1248.851	91.560	9

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(3)	2(2)					
1Br	2.36(2)	3(2)					
1Br	2.51(2)	4(2)					
1Imd	1.96(5)	4(5)	7(3)	0.1755	1462.344	107.213	9
0N/O							
1Br	2.33(2)	3(1)					
1Br	2.47(3)	5(2)					
1Imd	2.02(2)	3(1)					
1Imd	1.88(2)	1(2)	0(3)	0.1522	1268.301	92.986	9

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(4)	4(5)					
1Br	2.36(2)	3(2)					
1Br	2.51(2)	4(2)					
1Imd	2.07(2)	1(2)	8(3)	0.1602	1334.649	97.851	9
0N/O							
1Br	2.34(2)	3(2)					
1Br	2.47(3)	5(2)					
1Imd	1.88(2)	1(2)					
1Imd	2.02(2)	3(1)	0(3)	0.1541	1283.700	94.115	9

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(4)	4(5)					
1Br	2.36(2)	3(2)					
1Br	2.51(2)	4(2)					
1Imd	2.07(2)	1(2)	8(2)	0.1623	1351.861	99.113	9
0N/O							
1Br							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-Br(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(3)	2(2)					
1Br	2.51(2)	3(2)					
1Br	2.37(2)	3(2)					
1Imd	1.96(5)	4(5)	7(3)	0.1761	1466.881	107.545	9

0N/O							
1Br	2.48(3)	4(2)					
1Br	2.34(2)	3(2)					
1Imd	2.03(2)	3(1)					
1Imd	1.89(2)	1(2)	1(3)	0.1601	1333.832	97.791	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.94(4)	6(5)	neg2(2)	0.0506	478.600	35.089	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.88(1)	1(1)					
1Imd	2.02(2)	1(1)	0(1)	0.0395	328.815	24.107	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.42(2)	8(1)					
1Imd	1.94(4)	6(5)	neg2(2)	0.0512	426.227	31.249	9
1S	2.22(1)	2(1)					
1Br	2.42(2)	10(2)					
1Imd	1.88(1)	1(1)					
1Imd	2.02(2)	1(1)	0(1)	0.0404	336.752	24.689	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.42(2)	8(1)					
1Imd	1.94(4)	6(4)	neg2(2)	0.0513	427.486	31.341	9
1S	2.22(1)	2(1)					
1Br	2.42(2)	10(2)					
1Imd	2.02(2)	1(1)					
1Imd	1.88(1)	1(1)	0(2)	0.0412	343.541	25.187	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.42(2)	8(1)					
1Imd	1.94(5)	6(4)	neg2(2)	0.0514	427.955	31.376	9
1S	2.22(1)	2(1)					
1Br	2.42(2)	10(2)					
1Imd	2.02(2)	1(1)					
1Imd	1.88(1)	1(1)	1(2)	0.0420	349.578	25.630	9

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.93(4)	6(4)	neg3(2)	0.0508	423.340	31.037	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.87(1)	1(1)					
1Imd	2.02(2)	1(1)	0(1)	0.0390	325.136	23.838	9

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.93(4)	6(4)	neg3(2)	0.0514	427.953	31.376	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.87(1)	1(1)					
1Imd	2.02(2)	1(1)	0(1)	0.0399	332.714	24.393	9

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.94(4)	6(4)	neg3(2)	0.0515	429.008	31.453	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.87(1)	1(1)					
1Imd	2.02(2)	1(1)	0(2)	0.0407	339.148	24.865	9

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.94(4)	6(4)	neg3(2)	0.0515	429.289	31.474	9
1S	2.22(1)	2(1)					
1Br	2.42(2)	10(2)					
1Imd	2.02(2)	1(1)					
1Imd	1.87(1)	1(1)	0(2)	0.0414	344.898	25.286	9

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.93(4)	6(4)	neg3(2)	0.0508	422.877	31.003	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.87(1)	1(1)					
1Imd	2.02(2)	1(1)	0(1)	0.0387	322.841	23.669	9

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.93(4)	6(4)	neg3(2)	0.0513	427.111	31.314	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.87(1)	1(1)					
1Imd	2.02(2)	1(1)	0(1)	0.0396	330.010	24.195	9

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.93(4)	6(4)	neg3(2)	0.0514	427.882	31.370	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.87(1)	1(1)	0(1)	0.0403	336.096	24.641	9

1Imd	2.02(2)	1(1)					

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(3)	4(3)					
1S	2.20(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.93(4)	6(4)	neg3(2)	0.0514	427.878	31.370	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	2.02(2)	1(1)					
1Imd	1.87(1)	1(1)	0(1)	0.0410	341.541	25.040	9

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(4)	4(3)					
1S	2.19(1)	1(1)					
1Br	2.41(2)	8(1)					
1Imd	1.93(4)	6(4)	neg3(2)	0.0510	424.599	31.130	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	1.87(1)	1(1)					
1Imd	2.01(2)	1(1)	0(1)	0.0385	320.791	23.519	9

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(6)	7(9)					
1S	1.73(4)	18(6)					
1Br	2.45(2)	9(2)					
1Imd	2.11(1)	1(1)	13(2)	0.1542	1285.039	94.213	9
1S	2.22(1)	2(1)					
1Br	2.41(2)	10(2)					
1Imd	2.01(2)	1(1)					
1Imd	1.87(1)	1(1)	0(1)	0.0393	327.571	24.016	9

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.99(3)	1(3)					
1S	3.08(3)	1(2)					
1Br	2.44(2)	8(2)					
1Imd	2.10(2)	3(1)	10(3)	0.1772	1476.645	108.261	9

1S	3.04(4)	5(5)					
1Br	2.42(2)	7(2)					
1Imd	2.09(2)	4(1)					
1Imd	1.96(3)	1(2)	8(2)	0.1911	1592.382	116.747	9

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(5)	3(6)					
1S	2.77(4)	5(4)					
1Br	2.42(3)	8(3)					
1Imd	2.10(2)	2(1)	11(3)	0.2319	1932.207	141.661	9
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(5)	3(5)					
1S	2.76(4)	4(4)					
1Br	2.40(3)	7(2)					
1Imd	2.09(2)	2(1)	9(3)	0.2310	1924.795	141.118	9
1S	2.55(3)	2(2)					
1Br	2.24(2)	4(1)					
1Imd	1.83(3)	1(3)					
1Imd	1.74(9)	8(15)	neg26(5)	0.1552	1292.750	94.779	9

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.98(5)	3(5)					
1S	2.76(4)	4(4)					
1Br	2.40(3)	7(2)					
1Imd	2.09(2)	2(1)	9(3)	0.2342	1951.128	143.048	9
1S	3.05(4)	5(4)					
1Br	2.42(2)	7(2)					
1Imd	1.96(3)	1(2)					
1Imd	2.09(2)	4(1)	8(2)	0.1870	1556.859	114.142	9

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	2.02(5)	3(6)					
1S	2.80(8)	11(11)					
1Br	2.43(3)	8(3)					
1Imd	2.10(2)	1(1)	12(3)	0.2394	1994.488	146.227	9
1S	3.05(4)	5(5)					
1Br	2.42(2)	7(2)					
1Imd	2.09(2)	4(1)					
1Imd	1.96(3)	1(2)	8(2)	0.1898	1581.513	115.950	9

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(2)	5(2)					
1S	2.77(2)	6(2)					
1Br	2.73(2)	3(2)					
1Imd	1.99(3)	2(3)	9(3)	0.2512	2093.234	153.467	9
1S	2.93(0.22)	22(43)					
1Br	2.85(5)	8(5)					
1Imd	2.01(4)	1(6)					
1Imd	2.11(2)	3(2)	12(3)	0.3222	2684.302	196.801	9

Ni-S(2.2) Ni-S(2.3) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	7(7)					
1Br	2.39(2)	8(2)					
1Imd	1.87(3)	3(2)	neg8(3)	0.0521	434.402	31.848	9

Ni-S(2.2) Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	7(7)					
1Br	2.39(2)	8(2)					
1Imd	1.87(3)	3(2)	neg8(3)	0.0526	437.922	32.107	9

Ni-S(2.2) Ni-S(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	7(7)					
1Br	2.40(2)	8(2)					
1Imd	1.87(3)	3(2)	neg8(3)	0.0527	439.040	32.189	9

Ni-S(2.2) Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.10(5)	8(7)					
1S	2.19(1)	1(1)					
1Br	2.40(2)	8(2)					
1Imd	1.87(3)	3(2)	neg8(3)	0.0524	436.546	32.006	9

Ni-S(2.2) Ni-S(2.4) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.87(3)	3(2)	neg8(3)	0.0520	433.263	31.765	9

Ni-S(2.2) Ni-S(2.4) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(3)	3(2)	neg8(3)	0.0524	436.622	32.011	9

Ni-S(2.2) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	7(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(3)	3(2)	neg8(3)	0.0525	437.643	32.086	9

Ni-S(2.2) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	7(7)					
1Br	2.40(2)	8(2)					
1Imd	1.86(3)	3(2)	neg8(3)	0.0526	437.851	32.101	9

Ni-S(2.2) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.87(3)	3(2)	neg8(3)	0.0521	433.828	31.806	9

Ni-S(2.2) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(3)	3(2)	neg8(3)	0.0525	437.047	32.042	9

Ni-S(2.2) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(3)	3(2)	neg8(3)	0.0526	437.964	32.110	9

Ni-S(2.2) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.92(0.19)	28(35)					
1Br	2.40(2)	8(2)					
1Imd	1.89(2)	2(1)	neg4(3)	0.0811	675.829	49.549	9

Ni-S(2.2) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.96(0.22)	31(44)					
1Br	2.40(2)	7(2)					
1Imd	1.89(2)	2(1)	neg4(3)	0.0781	650.806	47.714	9

Ni-S(2.2) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0526	438.210	32.128	9

Ni-S(2.2) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(3)	3(2)	neg8(3)	0.0527	439.024	32.187	9

Ni-S(2.2) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.20(2)	1(1)					
1S	2.72(0.10)	4(1)					
1Br	2.70(9)	6(5)					
1Imd	1.91(3)	2(2)	neg5(4)	0.1264	1053.092	77.208	9

Ni-S(2.3) Ni-S(2.4) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0515	429.399	31.482	9

Ni-S(2.3) Ni-S(2.4) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.10(5)	8(7)					
1S	2.19(1)	1(1)					
1Br	2.39(2)	8(2)					
1Imd	1.87(2)	3(2)	neg8(3)	0.0516	430.002	31.526	9

Ni-S(2.3) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0520	433.152	31.757	9

Ni-S(2.3) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.10(5)	8(7)					
1S	2.19(1)	1(1)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0517	430.347	31.551	9

Ni-S(2.3) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.10(5)	8(7)					
1S	2.19(1)	1(1)					
1Br	2.39(2)	8(2)					
1Imd	1.87(2)	3(2)	neg8(3)	0.0514	428.418	31.410	9

Ni-S(2.3) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0520	433.045	31.749	9

Ni-S(2.3) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0520	433.665	31.794	9

Ni-S(2.3) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.93(0.19)	28(36)					
1Br	2.40(2)	8(2)					
1Imd	1.89(2)	2(1)	neg4(3)	0.0791	658.720	48.294	9

Ni-S(2.3) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.96(0.22)	31(42)					
1Br	2.40(2)	7(2)					
1Imd	1.89(2)	2(1)	neg4(3)	0.0762	634.514	46.520	9

Ni-S(2.3) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0521	434.263	31.838	9

Ni-S(2.3) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0522	434.785	31.877	9

Ni-S(2.3) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.94(0.20)	29(38)					
1Br	2.40(2)	8(2)					
1Imd	1.89(2)	2(1)	neg4(3)	0.0791	659.005	48.315	9

Ni-S(2.4) Ni-S(2.5) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.96(0.22)	30(42)					
1Br	2.40(2)	7(2)					
1Imd	1.89(2)	2(1)	neg5(3)	0.0746	621.891	45.594	9

Ni-S(2.4) Ni-S(2.5) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0516	429.982	31.524	9

Ni-S(2.4) Ni-S(2.5) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.93(0.21)	29(39)					
1S	2.18(1)	1(1)					
1Br	2.40(2)	8(2)					
1Imd	1.88(2)	2(1)	neg5(3)	0.0765	637.624	46.748	9

Ni-S(2.4) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.92(0.20)	28(38)					
1S	2.18(1)	1(1)					
1Br	2.40(2)	8(2)					
1Imd	1.88(2)	2(1)	neg5(3)	0.0771	642.763	47.125	9

Ni-S(2.4) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.97(0.22)	30(42)					
1Br	2.40(2)	7(2)					
1Imd	1.89(2)	2(1)	neg4(3)	0.0746	621.569	45.571	9

Ni-S(2.4) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.96(0.21)	30(41)					
1Br	2.40(2)	7(2)					
1Imd	1.89(2)	2(1)	neg4(3)	0.0759	632.079	46.341	9

Ni-S(2.4) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.10(5)	8(7)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0518	431.647	31.646	9

Ni-S(2.4) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.24(3)	2(3)					
1S	2.14(3)	2(3)					
1Br	2.81(5)	14(7)					
1Imd	1.86(2)	2(2)	neg6(2)	0.0750	624.906	45.815	9

Ni-S(2.5) Ni-S(2.6) Ni-Br(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.98(0.22)	31(43)					
1Br	2.40(2)	8(2)					
1Imd	1.88(2)	2(1)	neg5(3)	0.0743	618.725	45.362	9

Ni-S(2.5) Ni-S(2.6) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.10(5)	8(7)					
1S	2.19(1)	1(1)					
1Br	2.39(2)	8(2)					
1Imd	1.86(2)	3(2)	neg8(3)	0.0518	431.748	31.654	9

Ni-S(2.5) Ni-S(2.6) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.81(5)	5(6)					
1S	3.06(5)	3(5)					
1Br	2.43(3)	7(3)					
1Imd	2.09(2)	2(1)	14(3)	0.3140	2616.332	191.818	9

Ni-S(2.5) Ni-S(2.6) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	3.33(0.16)	9(18)					
1S	3.00(0.27)	18(46)					
1Br	2.88(6)	7(5)					
1Imd	2.11(2)	2(1)	17(4)	0.4502	3750.917	275.001	9

Table J.2. Additional Fits for Ni(II) WT-InrS in Buffer with 10 mM Hepes, 1 M NaOAc, 5 mM TCEP at 8.1.
Data Fit from k = 2 – 12.5 Å^{-1} and r = 1- 4 Å.

Ni-N(2.0)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.12(3)	1(2)	14(4)	0.4897	11255.513	670.057	3
3N/O	2.11(3)	4(2)	12(3)	0.4611	10598.298	630.932	3
4N/O	2.10(3)	6(2)	10(3)	0.4737	10888.029	648.180	3
5N/O	2.08(3)	9(3)	9(3)	0.5082	11680.804	695.375	3
6N/O	2.07(4)	11(3)	7(3)	0.5501	12642.393	752.620	3
7N/O	2.06(4)	14(4)	6(4)	0.5915	13594.945	809.326	3

Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.25(2)	5(1)	1(4)	0.2725	6262.307	372.804	3
3S	2.23(2)	7(1)	neg1(3)	0.2681	6161.145	366.782	3
4S	2.22(2)	10(1)	neg3(4)	0.2975	6838.567	407.110	3
5S	2.22(3)	12(2)	neg5(4)	0.3385	7780.844	463.205	3
6S	2.21(3)	15(2)	neg6(4)	0.3811	8759.846	521.486	3
7S	2.20(3)	17(2)	neg7(4)	0.4210	9676.824	576.075	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.04(2)	2(2)					
1N/O	2.17(2)	6(1)	10(3)	0.3151	7241.716	489.376	5
2N/O	2.00(3)	0(3)					
2N/O	2.15(2)	2(2)	8(3)	0.3932	9036.243	610.646	5
3N/O	2.04(2)	2(2)					
1N/O	2.17(2)	5(2)	9(3)	0.3638	8361.970	565.080	5
4N/O	2.03(3)	6(4)					
1N/O	2.16(3)	3(2)	7(3)	0.4173	9590.515	648.102	5
3N/O	1.99(5)	7(6)					
2N/O	2.13(3)	0(3)	6(3)	0.4362	10025.649	677.507	5

5N/O	2.02(5)	12(5)					
1N/O	2.13(3)	2(2)	6(4)	0.4584	10536.215	712.010	5
4N/O	2.09(3)	4(3)					
2N/O	1.92(7)	9(11)	6(4)	0.4520	10388.055	701.998	5
3N/O	1.94(8)	16(14)					
3N/O	2.10(3)	3(3)	4(4)	0.4631	10642.541	719.195	5
6N/O	2.07(4)	9(3)					
1N/O	1.82(8)	6(10)	6(4)	0.4866	11182.772	755.702	5
5N/O	2.08(3)	6(3)					
2N/O	1.87(7)	11(12)	5(4)	0.4651	10688.502	722.301	5
4N/O	2.09(3)	5(3)					
3N/O	1.92(7)	15(13)	4(4)	0.4594	10558.664	713.527	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.15(2)	4(2)					
1S	2.27(2)	1(1)	neg5(3)	0.1817	4176.341	282.226	5
2S	2.11(3)	7(3)					
2S	2.25(2)	3(2)	neg7(4)	0.2245	5159.014	348.633	5
3S	2.23(2)	4(1)					
1S	2.07(3)	3(3)	neg6(3)	0.2258	5189.300	350.679	5
4S	2.21(3)	7(2)					
1S	2.03(4)	6(5)	neg7(4)	0.2569	5903.696	398.956	5
3S	2.23(2)	5(2)					
2S	2.08(4)	10(5)	neg8(4)	0.2438	5603.736	378.686	5
5S	2.20(3)	10(2)					
1S	1.98(5)	8(5)	neg8(4)	0.2787	6405.853	432.891	5
4S	2.21(2)	7(2)					
2S	2.03(5)	12(6)	neg9(4)	0.2606	5990.281	404.807	5
3S	2.06(5)	17(7)					
3S	2.22(2)	6(2)	neg10(4)	0.2581	5932.321	400.891	5
6S	2.19(3)	12(2)					
1S	1.95(4)	8(5)	neg9(4)	0.3001	6897.543	466.118	5
5S	2.20(3)	9(2)	neg10(4)	0.2759	6341.074	428.513	5

2S	2.00(4)	12(6)					
4S	2.21(2)	8(2)					
3S	2.04(4)	16(7)	neg10(4)	0.2657	6106.677	412.673	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.02(3)	3(2)					5
1S	2.28(2)	0(1)	6(3)	0.1878	4315.980	291.663	
1N/O	1.97(4)	1(3)					5
2S	2.25(2)	4(1)	1(4)	0.2202	5060.611	341.983	
2N/O	2.17(6)	12(16)					
2S	2.27(2)	5(2)	10(0)	0.2229	5123.255	346.216	5
3N/O	2.05(6)	10(4)					
1S	2.27(2)	1(1)	7(5)	0.2096	4816.904	325.514	5
1N/O	2.13(0.41)	33(216)					
3S	2.24(3)	7(2)	0(8)	0.2614	6007.057	405.941	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.09(0.10)	17(6)					
1S	2.27(2)	1(1)	8(6)	0.2207	5073.236	342.836	5
2N/O	2.20(2)	4(1)					
3S	2.20(2)	2(1)	neg1(4)	0.1698	3903.543	263.791	5
3N/O	2.21(5)	16(18)					
2S	2.28(2)	4(1)	12(5)	0.1965	4516.251	305.196	5
5N/O	2.12(0.11)	23(9)					
1S	2.27(2)	1(1)	9(6)	0.2279	5237.167	353.914	5
1N/O	2.41(1)	4(1)					
5S	2.19(4)	16(2)	neg9(4)	0.1831	4207.673	284.344	5
4N/O	2.24(4)	21(13)					
2S	2.28(1)	4(1)	13(4)	0.1764	4054.128	273.967	5
2N/O	2.41(1)	1(1)					
4S	2.19(4)	15(2)	neg10(5)	0.1557	3578.422	241.820	5
3N/O	2.24(2)	3(2)					
3S	2.24(2)	2(1)	10(3)	0.1618	3719.028	251.322	5

6N/O	2.16(0.10)	31(12)					
1S	2.28(2)	1(1)	10(6)	0.2302	5290.894	357.545	5
1N/O	2.41(2)	4(1)					
6S	2.19(4)	18(2)	neg9(5)	0.2028	4659.922	314.905	5
5N/O	2.25(4)	25(10)					
2S	2.29(1)	4(1)	13(3)	0.1623	3730.601	252.104	5
2N/O	2.41(1)	1(1)					
5S	2.19(5)	18(3)	neg10(5)	0.1681	3863.234	261.067	5
4N/O	2.25(2)	3(1)					
3S	2.24(2)	0(1)	12(2)	0.1365	3136.548	211.960	5
3N/O	2.20(2)	2(1)					
4S	2.20(2)	4(1)	neg1(4)	0.1771	4070.364	275.065	5

Ni-N(2.0) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	3(2)					5
1Br	2.40(2)	4(1)	6(4)	0.1565	3598.007	243.144	
1N/O	2.00(4)	1(3)					5
2Br	2.37(2)	7(1)	neg2(6)	0.1982	4554.162	307.758	
2N/O	2.04(3)	4(2)					
2Br	2.40(2)	8(1)	5(4)	0.1482	3405.894	230.161	5
3N/O	2.05(3)	6(2)					
1Br	2.40(1)	4(1)	6(3)	0.1372	3152.739	213.054	5
1N/O	1.97(4)	2(3)					
3Br	2.37(2)	9(1)	neg5(6)	0.1935	4447.432	300.546	5
1N/O	1.88(8)	8(8)					
4Br	2.33(3)	11(1)	neg13(6)	0.1970	4526.707	305.903	5
4N/O	2.05(3)	9(2)					
1Br	2.40(1)	4(1)	5(3)	0.1429	3283.696	221.904	5
2N/O	2.04(4)	6(3)					
3Br	2.40(2)	10(1)	4(4)	0.1551	3564.490	240.879	5
3N/O	2.05(3)	8(2)					
2Br	2.40(2)	8(1)	5(3)	0.1284	2951.893	199.481	5
5N/O	2.04(3)	12(3)					
1Br	2.39(1)	4(1)	4(3)	0.1574	3617.966	244.493	5

1N/O	1.08(3)	3(4)					
5Br	2.34(2)	13(1)	neg12(5)	0.2108	4845.415	327.440	5
4N/O	2.04(3)	11(3)					
2Br	2.40(1)	8(1)	4(3)	0.1275	2930.969	298.067	5
2N/O	2.05(4)	6(3)					
4Br	2.41(2)	13(1)	5(4)	0.1666	3828.246	258.703	5
3N/O	2.05(3)	9(3)					
3Br	2.40(2)	11(1)	5(4)	0.1351	3105.245	209.844	5
6N/O	2.03(4)	16(3)					
1Br	2.39(1)	4(1)	3(4)	0.1722	3958.616	267.513	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.03(4)	15(3)					
2Br	2.39(1)	8(1)	2(4)	0.1321	3035.997	205.165	5
2N/O	1.82(6)	13(8)					
5Br	2.32(2)	12(1)	neg16(5)	0.1706	3920.848	264.961	5
4N/O	2.03(4)	13(3)					
3Br	2.40(2)	10(1)	3(4)	0.1308	3006.681	203.184	5
3N/O	2.06(3)	9(3)					
4Br	2.41(2)	13(1)	5(3)	0.1464	3364.217	227.345	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.05(5)	13(6)					
1Imd	2.13(4)	1(3)	8(4)	0.4682	18090.014	1222.476	5
4N/O	1.99(6)	18(10)					
1Imd	2.16(2)	6(2)					
1Imd	2.03(2)	5(2)	7(3)	0.3507	8060.202	629.809	7
3N/O	1.95(0.12)	25(23)					
1Imd	2.03(4)	9(3)					
1Imd	1.91(5)	4(6)					
1Imd	2.15(3)	9(3)	4(3)	0.3137	7209.419	667.672	9
2N/O	2.06(5)	4(6)					
1Imd	2.02(5)	7(4)					
1Imd	2.16(4)	7(3)					
1Imd	1.86(6)	1(8)	8(4)	0.2642	6071.714	690.136	11

1Imd	1.59(0.13)	15(21)					
1N/O	2.08(4)	2(4)					
1Imd	1.76(6)	8(6)					
1Imd	1.55(0.10)	5(11)					
1Imd	2.16(3)	14(2)					
1Imd	1.90(4)	15(4)					
1Imd	2.02(3)	16(3)	6(4)	0.1791	4116.258	605.523	13
4N/O	2.06(4)	9(5)					
1Imd	2.15(4)	0(3)	9(3)	0.4369	10040.443	678.507	5
3N/O	2.00(6)	14(10)					
1Imd	2.03(3)	5(2)					
1Imd	2.17(2)	6(2)	8(3)	0.3391	7794.043	609.012	7
2N/O	2.06(5)	4(6)					
1Imd	2.15(3)	7(2)					
1Imd	1.87(5)	2(5)					
1Imd	2.01(4)	7(3)	6(3)	0.2965	6815.155	631.158	9
1N/O	2.07(4)	2(4)					
1Imd	2.02(2)	17(2)					
1Imd	2.14(2)	14(2)					
1Imd	1.90(3)	16(2)					
1Imd	1.79(3)	9(3)	1(3)	0.2136	4909.794	558.067	11
0N/O							
1Imd	1.53(0.11)	8(16)					
1Imd	1.80(7)	5(8)					
1Imd	1.92(4)	14(4)					
1Imd	2.17(3)	14(2)					
1Imd	2.04(3)	16(3)	6(4)	0.2518	5788.089	657.898	11
3N/O	2.06(3)	5(4)					
1Imd	2.17(4)	1(3)	11(3)	0.4107	9439.536	637.899	5
2N/O	2.02(7)	9(11)					
1Imd	2.17(2)	6(2)					
1Imd	2.04(3)	5(2)	9(3)	0.3333	7660.001	598.538	7
1N/O	2.08(5)	0(6)					
1Imd	1.90(5)	3(5)					
1Imd	2.16(3)	8(2)					
1Imd	2.03(4)	8(3)	7(3)	0.2845	6539.710	605.649	9
0N/O							
1Imd	2.03(2)	17(2)					
1Imd	1.81(3)	9(3)					
1Imd	2.15(2)	15(2)	1(3)	0.2644	6076.460	562.747	9

1Imd	1.92(3)	15(2)					
2N/O	2.07(3)	2(4)					
1Imd	2.18(3)	2(3)	14(3)	0.4122	9472.564	640.131	5
1N/O	2.10(5)	1(5)					
1Imd	2.03(3)	3(2)					
1Imd	2.18(3)	5(2)	12(2)	0.3280	7538.641	589.055	7
0N/O							
1Imd	2.16(2)	9(2)					
1Imd	1.93(4)	4(5)					
1Imd	2.04(3)	9(3)	7(3)	0.3353	7705.721	602.111	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.94(0.10)	18(14)					
1S	2.26(2)	0(1)					
1Imd	2.01(3)	0(2)	2(4)	0.1639	3766.151	294.280	7
1N/O	1.91(0.22)	18(36)					
1S	2.25(2)	1(1)					
1Imd	1.87(8)	5(10)					
1Imd	2.00(3)	2(2)	neg1(3)	0.1591	3657.587	338.733	9

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.94(0.11)	18(14)					
1S	2.26(2)	0(1)					
1Imd	2.01(3)	0(2)	2(4)	0.1622	3726.980	291.219	7
1N/O	1.97(3)	3(2)					
1S	2.25(2)	2(1)					
1Imd	1.81(3)	0(3)					
1Imd	1.98(5)	1(4)	neg3(3)	0.1312	3014.855	279.209	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.15(0.13)	26(31)					
1S	2.28(2)	0(1)					
1Imd	2.03(3)	1(2)	7(4)	0.1621	3724.778	291.047	7
1N/O	2.23(0.24)	26(54)					
1S	2.28(2)	1(2)					
1Imd	2.04(3)	2(2)					
1Imd	2.20(3)	3(3)	11(2)	0.1307	3003.572	278.164	9

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	3(4)					
1S	2.70(5)	6(6)					
1Imd	2.16(4)	1(3)	11(3)	0.3406	7827.865	611.655	7
1N/O	2.10(3)	3(3)					
1S	2.66(3)	2(3)					
1Imd	2.16(3)	5(2)					
1Imd	2.00(2)	4(2)	9(2)	0.2445	5620.294	520.501	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(3)	2(4)					
1S	2.71(5)	6(6)					
1Imd	2.17(4)	2(3)	12(3)	0.3468	7970.297	622.784	7
1N/O	2.10(4)	2(4)					
1S	2.66(3)	2(3)					
1Imd	2.00(3)	4(2)					
1Imd	2.16(3)	5(2)	9(2)	0.2544	5846.815	541.479	9

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.22(0.11)	36(31)					
1S	2.28(1)	0(1)					
1Imd	2.03(3)	1(2)	9(3)	0.1607	3694.281	288.664	7
2N/O	1.94(0.11)	21(15)					
1S	2.23(2)	2(2)					
1Imd	2.46(2)	2(1)					
1Imd	1.99(4)	3(4)	neg1(3)	0.088	2022.781	187.332	9

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.21(0.10)	33(27)					
1S	2.29(1)	0(1)					
1Imd	2.04(3)	1(2)	9(3)	0.1561	3586.609	280.251	7
2N/O	1.95(0.11)	22(16)					
1S	2.23(2)	2(2)					
1Imd	1.99(5)	4(4)					
1Imd	2.46(2)	2(1)	neg2(4)	0.0894	2054.688	190.287	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.21(9)	21(24)					
1S	2.29(1)	0(1)					
1Imd	2.04(3)	1(2)	9(3)	0.1529	3515.010	274.656	7
2N/O	2.27(0.15)	34(35)					
1S	2.28(2)	1(2)					
1Imd	2.04(3)	2(2)					
1Imd	2.20(3)	2(3)	12(2)	0.121	2779.847	257.444	9

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(3)	6(4)					
1S	2.67(4)	4(4)					
1Imd	2.15(4)	1(3)	9(3)	0.317	7285.519	569.277	7
2N/O	1.97(6)	10(9)					
1S	2.66(3)	2(3)					
1Imd	2.15(2)	7(2)					
1Imd	2.02(2)	6(2)	7(2)	0.2087	4796.556	444.214	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(3)	6(4)					
1S	2.68(4)	5(4)					
1Imd	2.15(4)	1(3)	9(3)	0.3246	7460.523	582.951	7
2N/O	1.97(6)	10(9)					
1S	2.67(3)	3(3)					
1Imd	2.02(2)	6(2)					
1Imd	2.15(2)	7(2)	6(2)	0.2138	4914.453	455.132	9

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.43(2)	4(1)					
2S	2.18(2)	5(1)					
1Imd	1.85(6)	7(5)	neg10(4)	0.1011	2324.033	181.596	7
0N/O							
2S	2.23(2)	3(1)					
1Imd	1.95(2)	2(2)					
1Imd	1.80(3)	1(3)	neg5(3)	0.1539	3536.820	276.360	9

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.79(5)	6(7)					
2S	2.24(2)	4(1)					
1Imd	1.96(3)	0(2)	neg3(3)	0.1756	4036.968	315.441	7
0N/O							
2S	2.23(2)	3(1)					
1Imd	1.80(3)	1(3)					
1Imd	1.95(2)	2(2)	neg5(3)	0.1518	3489.324	272.649	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.19(2)	7(1)					
2S	2.19(2)	1(1)					
1Imd	1.87(4)	4(4)	neg7(4)	0.1139	2617.467	204.524	7
0N/O							
2S	2.23(2)	3(1)					
1Imd	1.79(3)	1(3)					
1Imd	1.94(2)	2(2)	neg6(3)	0.1517	3486.942	272.463	9

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.13(3)	5(2)					
2S	2.67(4)	6(3)					
1Imd	2.01(3)	3(2)	6(4)	0.4077	9370.967	732.230	7
0N/O							
2S	2.70(4)	8(4)					
1Imd	2.16(2)	7(2)					
1Imd	2.03(2)	6(2)	10(2)	0.3628	8338.885	651.585	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(5)	0(6)					
2S	2.75(6)	13(8)					
1Imd	2.16(4)	2(4)	13(3)	0.4436	10194.720	796.596	7
0N/O							
2S	2.70(3)	9(5)					
1Imd	2.03(2)	6(2)					
1Imd	2.16(1)	7(2)	10(0)	0.3756	8631.384	674.440	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.35(0.26)	0(40)					
1S	2.13(5)	3(4)					
1S	2.27(9)	4(5)					
1Imd	1.85(6)	3(5)	neg8(5)	0.0989	2272.908	210.496	9
0N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(3)	6(2)					
1S	2.25(2)	3(2)					
1S	2.07(5)	5(9)					
1Imd	1.89(6)	3(5)	neg4(4)	0.1069	2457.617	227.602	9
0N/O							
1S	2.27(2)	3(1)					
1S	2.13(2)	2(2)					
1Imd	1.97(7)	4(9)					
1Imd	1.81(4)	3(5)	neg6(3)	0.0984	2262.475	209.530	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(7)	9(9)					
1S	2.25(2)	0(1)					
1S	2.63(2)	3(2)					
1Imd	1.99(3)	0(2)	0(3)	0.0748	1718.538	159.156	9
0N/O							
1S	2.23(2)	0(1)					
1S	2.62(2)	2(2)					
1Imd	1.83(5)	6(6)					
1Imd	1.97(3)	2(2)	neg4(4)	0.0827	1900.498	176.007	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(7)	9(9)					
1S	2.25(2)	0(1)					
1S	2.63(2)	3(2)					
1Imd	1.99(3)	0(2)	neg1(3)	0.0758	1741.294	161.263	9

0N/O							
1S	2.23(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.83(5)	6(6)					
1Imd	1.97(3)	2(2)	neg4(3)	0.0843	1937.305	179.416	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.17(6)	8(5)					
1S	2.32(3)	2(4)					
1S	2.16(4)	5(4)					
1Imd	2.10(6)	4(7)	8(3)	0.1368	3144.952	291.257	9
0N/O							
1S	2.23(2)	0(1)					
1S	2.61(2)	2(2)					
1Imd	1.82(5)	5(5)					
1Imd	1.97(3)	2(2)	neg5(4)	0.081	1862.758	172.512	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(7)	10(10)					
1S	2.25(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	2.00(3)	0(2)	neg1(3)	0.0759	1743.336	161.452	9
0N/O							
1S	2.23(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.83(5)	6(6)					
1Imd	1.97(3)	2(2)	neg4(4)	0.0818	1880.751	174.178	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(7)	10(10)					
1S	2.25(2)	0(1)					
1S	2.63(2)	3(2)					
1Imd	2.00(3)	0(2)	neg1(3)	0.0766	1759.874	162.984	9
0N/O							
1S	2.24(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.97(3)	2(2)					
1Imd	1.83(5)	6(6)	neg4(4)	0.0832	1912.014	177.074	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.90(8)	10(11)					
1S	2.62(2)	3(2)					
1S	2.25(2)	0(1)					
1Imd	2.00(3)	0(2)	neg1(4)	0.0787	1808.170	167.456	9
0N/O							
1S	2.66(3)	2(3)					
1S	2.64(5)	20(9)					
1Imd	2.15(2)	7(1)					
1Imd	2.01(2)	6(2)	7(2)	0.2278	5236.219	484.932	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(7)	10(10)					
1S	2.25(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.99(3)	0(2)	neg1(4)	0.0776	1783.378	165.160	9
0N/O							
1S	2.24(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.82(5)	5(5)					
1Imd	1.97(3)	2(2)	neg4(4)	0.0828	1903.199	176.257	9

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(3)	7(2)					
1S	2.67(4)	1(3)					
1S	2.91(7)	3(8)					
1Imd	1.99(3)	5(2)	7(4)	0.2563	5890.525	545.528	9
0N/O							
1S	2.70(4)	4(4)					
1S	3.05(7)	6(9)					
1Imd	2.17(2)	7(1)					
1Imd	2.03(2)	6(2)	12(2)	0.2675	6148.609	569.429	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.35(0.12)	1(24)					
1S	2.13(4)	2(4)					
1S	2.28(8)	4(4)					
1Imd	1.85(6)	3(5)	neg10(4)	0.0943	3641.957	337.285	9

1N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.18(5)	5(6)					
1S	2.16(4)	4(4)					
1S	2.30(2)	1(3)					
1Imd	2.12(6)	5(7)	10(2)	0.107	2458.527	227.687	9
1N/O	2.27(4)	9(5)					
1S	2.26(3)	7(3)					
1S	2.14(3)	3(3)					
1Imd	1.82(8)	4(11)					
1Imd	1.96(0.11)	4(16)	neg7(4)	0.0874	2009.636	228.424	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(5)	15(7)					
1S	2.25(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.99(2)	0(1)	neg1(3)	0.0618	1419.231	131.436	9
1N/O	1.87(6)	6(6)					
1S	2.25(1)	1(1)					
1S	2.64(2)	3(2)					
1Imd	2.13(4)	2(4)					
1Imd	1.99(3)	3(2)	2(3)	0.0601	1381.230	156.996	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.89(5)	15(7)					
1S	2.25(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.99(2)	0(1)	neg1(3)	0.0625	1435.309	132.925	9
1N/O	1.87(6)	5(6)					
1S	2.25(1)	1(1)					
1S	2.64(2)	3(2)					
1Imd	2.13(4)	2(4)					
1Imd	1.98(3)	3(2)	1(3)	0.0613	1409.991	160.265	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.42(7)	9(15)					
1S	1.77(6)	22(9)					
1S	2.31(2)	1(2)					
1Imd	2.09(4)	2(3)	13(3)	0.1283	2948.827	273.094	9
1N/O	2.13(9)	8(11)					
1S	2.31(3)	3(6)					
1S	2.14(8)	4(9)					
1Imd	2.21(6)	2(8)					
1Imd	2.06(5)	1(9)	10(3)	0.1114	2559.461	290.919	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(6)	15(8)					
1S	2.25(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.99(2)	0(1)	neg1(3)	0.0631	1449.117	134.204	9
1N/O	1.87(6)	6(6)					
1S	2.25(2)	1(1)					
1S	2.63(2)	3(2)					
1Imd	1.99(3)	3(2)					
1Imd	2.13(4)	1(4)	2(3)	0.0614	1410.118	160.280	11

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(5)	15(7)					
1S	2.25(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.99(2)	0(1)	neg2(3)	0.0635	1460.432	135.252	9
1N/O	1.87(6)	6(6)					
1S	2.25(1)	1(1)					
1S	2.64(2)	3(2)					
1Imd	2.13(4)	2(4)					
1Imd	1.98(3)	3(2)	1(3)	0.0623	1432.021	162.769	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.91(6)	16(8)					
1S	2.61(2)	3(2)					
1S	2.25(2)	0(1)					
1Imd	2.00(3)	0(2)	neg2(4)	0.0658	1512.303	140.056	9

1N/O	1.88(7)	7(8)					
1S	2.63(2)	3(2)					
1S	2.25(2)	1(2)					
1Imd	1.99(3)	3(2)					
1Imd	2.13(5)	1(4)	2(3)	0.064	1470.826	167.180	11

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(6)	15(8)					
1S	2.25(2)	0(1)					
1S	2.62(2)	3(2)					
1Imd	1.99(2)	0(1)	neg2(3)	0.0646	1485.596	137.583	9
1N/O	1.95(6)	3(6)					
1S	2.24(2)	0(1)					
1S	2.63(2)	3(3)					
1Imd	1.78(4)	3(4)					
1Imd	1.97(3)	1(2)	neg4(4)	0.0614	1410.371	160.309	11

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.90(6)	16(8)					
1S	2.62(2)	3(2)					
1S	2.25(2)	1(1)					
1Imd	1.99(2)	0(2)	neg2(3)	0.0651	1496.781	138.618	9
1N/O	2.05(3)	5(3)					
1S	2.63(2)	4(2)					
1S	2.81(3)	3(3)					
1Imd	1.95(4)	2(5)					
1Imd	2.14(2)	5(2)	7(3)	0.1704	3915.225	445.021	11

Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.12(2)	1(2)					
1S	2.26(2)	3(1)					
1Imd 0°	1.82(5)	3(4)					
1Imd 5°	2.01(7)	2(7)	neg6(3)	0.1024	4125.477	382.065	9

Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.26(2)	3(1)					
1S	2.13(2)	2(2)					
1Imd 0°	1.83(5)	2(4)	neg6(3)	0.0957	3856.752	357.178	9

1Imd 5°	2.02(6)	1(6)					

Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	1(1)					
1S	2.62(2)	2(2)					
1Imd 0°	1.96(3)	3(2)					
1Imd 5°	1.81(4)	3(4)	neg5(3)	0.0797	3210.149	297.295	9

Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	1(1)					
1S	2.62(2)	2(2)					
1Imd 0°	1.96(3)	3(2)					
1Imd 5°	1.81(4)	3(4)	neg4(3)	0.0811	3268.835	302.730	9

Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.13(3)	0(2)					
1S	2.26(3)	1(3)					
1Imd 0°	1.19(0.19)	30(42)					
1Imd 5°	2.42(4)	1(4)	neg7(3)	0.1156	4657.487	431.335	9

Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.62(2)	2(2)					
1Imd 0°	1.96(3)	2(2)					
1Imd 5°	1.81(4)	3(4)	neg5(3)	0.0795	3204.625	296.784	9

Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.62(2)	2(2)					
1Imd 0°	1.96(3)	2(2)					
1Imd 5°	1.81(4)	3(4)	neg5(3)	0.0807	3253.909	301.348	9

Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.62(2)	2(2)	neg5(4)	0.0798	3214.484	297.697	9

1Imd 0°	1.96(3)	2(2)					
1Imd 5°	1.80(4)	3(4)					

Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.25(2)	0(1)					
1S	2.62(2)	4(3)					
1Imd 0°	1.85(7)	7(9)					
1Imd 5°	1.99(3)	1(3)	neg3(4)	0.0938	3779.521	350.025	9

Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.11(2)	1(1)					
1S	2.26(1)	4(1)					
1Imd 0°	1.82(2)	3(3)					
1Imd 10°	2.03(2)	3(2)	neg6(2)	0.0559	2253.429	208.692	9

Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.26(1)	4(1)					
1S	2.11(1)	1(1)					
1Imd 0°	1.83(2)	3(3)					
1Imd 10°	2.03(2)	2(2)	neg5(2)	0.0526	2118.179	196.167	9

Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	0(1)					
1S	2.61(2)	0(2)					
1Imd 0°	1.96(3)	2(1)					
1Imd 10°	1.80(4)	4(4)	neg5(4)	0.0815	3285.569	304.280	9

Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.61(2)	1(2)					
1Imd 0°	1.96(3)	2(1)					
1Imd 10°	1.81(4)	4(4)	neg5(4)	0.0826	3330.106	308.404	9

Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	1.55(6)	22(9)	neg2(3)	0.1188	4786.047	443.241	9

1S	2.26(2)	1(1)					
1Imd 0°	1.96(9)	8(9)					
1Imd 10°	1.99(3)	1(2)					

Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	0(1)					
1S	2.61(2)	0(2)					
1Imd 0°	1.95(3)	2(1)					
1Imd 10°	1.80(4)	4(4)	neg6(4)	0.0823	3318.497	307.329	9

Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	0(1)					
1S	2.61(2)	1(2)					
1Imd 0°	1.96(3)	2(1)					
1Imd 10°	1.80(4)	4(4)	neg5(4)	0.0832	3354.411	310.655	9

Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.62(3)	2(3)					
1S	2.24(2)	0(1)					
1Imd 0°	1.98(3)	0(2)					
1Imd 10°	1.86(8)	9(10)	neg3(4)	0.0856	3450.409	319.546	9

Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.22(2)	0(1)					
1S	2.61(2)	1(2)					
1Imd 0°	1.95(3)	2(1)					
1Imd 10°	1.79(4)	3(4)	neg6(4)	0.0839	3380.821	313.101	9

Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.11(2)	1(2)					
1S	2.26(1)	4(1)					
1Imd 5°	1.82(3)	3(3)					
1Imd 10°	2.03(2)	3(2)	neg5(2)	0.0628	2531.181	234.415	9

Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1S	2.26(1)	4(1)					
1S	2.12(2)	1(2)					
1Imd 5°	1.83(3)	3(3)					
1Imd 10°	2.03(2)	3(2)	neg5(2)	0.0589	2373.851	219.845	9

Ni-S(2.2) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.61(2)	1(2)					
1Imd 5°	1.96(3)	2(2)					
1Imd 10°	1.81(5)	4(5)	neg5(4)	0.0898	3620.145	335.265	9

Ni-S(2.2) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.61(3)	1(2)					
1Imd 5°	1.97(3)	2(2)					
1Imd 10°	1.82(5)	5(5)	neg4(4)	0.0912	3676.535	340.488	9

Ni-S(2.3) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.62(3)	5(4)					
1S	2.27(2)	1(1)					
1Imd 5°	1.99(7)	5(6)					
1Imd 10°	2.03(7)	3(6)	2(3)	0.0941	3791.465	351.131	9

Ni-S(2.3) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.61(3)	1(2)					
1Imd 5°	1.96(3)	2(2)					
1Imd 10°	1.80(5)	4(5)	neg6(4)	0.0895	3607.704	334.113	9

Ni-S(2.3) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.61(3)	1(2)					
1Imd 5°	1.96(3)	2(2)					
1Imd 10°	1.81(5)	4(5)	neg5(4)	0.0907	3655.883	338.575	9

Ni-S(2.4) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.63(3)	6(4)					
1S	2.27(2)	1(1)					
1Imd 5°	1.99(7)	5(6)					
1Imd 10°	2.03(7)	3(6)	2(3)	0.0953	3842.435	355.852	9

Ni-S(2.4) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(2)	0(1)					
1S	2.61(3)	1(2)					
1Imd 5°	1.96(3)	2(2)					
1Imd 10°	1.80(5)	4(4)	neg6(4)	0.0906	3652.374	338.250	9

Ni-S(2.5) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.63(3)	4(2)					
1S	2.80(3)	5(2)					
1Imd 5°	2.13(3)	4(3)					
1Imd 10°	2.01(3)	3(3)	7(3)	0.2606	10500.393	972.452	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.43(1)	6(1)					
1S	2.13(0.12)	14(27)					
1S	2.26(0.10)	8(12)					
1Imd 5°	1.88(4)	5(5)					
1Imd 10°	2.02(2)	3(1)	neg5(3)	0.0428	1723.919	195.948	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(4)	10(3)					
1S	2.28(2)	5(2)					
1S	2.07(3)	6(4)					
1Imd 5°	2.16(6)	5(8)					
1Imd 10°	2.07(2)	4(2)	6(2)	0.0504	2030.345	230.777	11

Ni-N(2.2) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.23(4)	9(2)					
1S	2.12(3)	2(7)					
1S	2.23(3)	5(3)					
1Imd 5°	1.87(5)	5(4)	neg3(3)	0.0477	1923.004	218.576	11

1Imd 10°	2.03(2)	3(1)					

Ni-N(2.2) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.23(5)	9(2)					
1S	2.23(4)	6(4)					
1S	2.13(3)	2(8)					
1Imd 5°	1.87(5)	5(4)					
1Imd 10°	2.03(2)	3(2)	neg3(3)	0.0489	1970.340	223.957	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.43(1)	6(1)					
1S	2.14(0.19)	13(34)					
1S	2.26(0.17)	9(18)					
1Imd 0°	1.87(4)	5(4)					
1Imd 10°	2.02(2)	3(1)	neg5(3)	0.0386	1554.786	176.723	11

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(2)	8(2)					
1S	2.25(1)	5(1)					
1S	2.04(2)	3(3)					
1Imd 0°	1.88(4)	5(4)					
1Imd 10°	2.03(2)	3(1)	neg3(2)	0.038	1529.405	173.838	11

Ni-N(2.2) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.23(4)	9(2)					
1S	2.12(3)	1(6)					
1S	2.24(3)	6(3)					
1Imd 0°	1.86(4)	4(4)					
1Imd 10°	2.03(2)	3(1)	neg4(3)	0.0435	1753.549	199.316	11

Ni-N(2.2) Ni-S(2.2) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.23(5)	9(2)					
1S	2.24(4)	6(4)					
1S	2.13(3)	1(7)					
1Imd 0°	1.86(4)	4(4)					
1Imd 10°	2.03(2)	3(2)	neg4(3)	0.045	1812.246	205.987	11

Table J.3. Additional Fits for Cu(II) WT-InrS in Buffer with 10 mM Hepes, 1 M NaBr, 5 mM TCEP at 8.1.
Data Fit from k = 2 - 14 $Å^{-1}$ and r = 1- 4 Å.

Cu-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(1)	1(1)	16(2)	0.2367	1128.920	57.482	3
3N/O	2.13(1)	2(1)	16(2)	0.1622	836.163	42.575	3
4N/O	2.12(1)	4(1)	14(1)	0.1649	850.350	43.298	3
5N/O	2.12(1)	6(1)	13(1)	0.2155	1111.305	56.585	3
6N/O	2.11(2)	7(1)	12(2)	0.2932	1511.765	76.975	3
7N/O	2.11(2)	10(2)	11(2)	0.3813	1965.833	100.095	3

Cu-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.23(1)	4(1)	neg1(2)	0.0926	477.649	24.321	3
3S	2.23(1)	6(0)	neg2(1)	0.0406	209.240	10.654	3
4S	2.23(1)	9(0)	neg2(1)	0.0471	242.690	12.357	3
5S	2.23(1)	11(1)	neg3(1)	0.0804	414.450	21.103	3
6S	2.23(1)	13(1)	neg3(2)	0.1250	644.635	32.823	3
7S	2.23(2)	15(1)	neg3(2)	0.1732	893.224	45.481	3

Cu-N(2.0) Cu-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.16(1)	2(1)					
1N/O	2.05(1)	3(1)	15(2)	0.1369	705.836	40.014	5
2N/O	2.06(4)	5(6)					
2N/O	2.14(3)	1(2)	12(2)	0.1628	839.257	47.578	5
3N/O	2.08(2)	3(3)					
1N/O	2.17(3)	1(2)	13(2)	0.1565	806.914	45.744	5
4N/O	2.08(3)	8(3)					
1N/O	2.14(3)	0(2)	11(2)	0.1986	1023.944	58.048	5
3N/O	2.05(5)	11(6)					
2N/O	2.13(2)	1(1)	10(2)	0.1977	1019.298	57.785	5
5N/O	2.08(3)	12(4)					
1N/O	2.13(2)	1(1)	10(2)	0.2485	1281.411	72.644	5
4N/O	2.13(1)	4(1)					
2N/O	1.65(8)	57(22)	17(2)	0.1286	662.987	37.585	5

3N/O	2.11(1)	2(1)					
3N/O	2.00(5)	16(9)	9(2)	0.2083	1074.047	60.888	5
6N/O	2.07(4)	17(5)					
1N/O	2.12(2)	1(1)	9(2)	0.2974	1533.672	86.945	5
5N/O	2.12(1)	5(1)					
2N/O	1.73(9)	44(18)	14(2)	0.1592	820.746	46.528	5
4N/O	2.13(1)	4(1)					
3N/O	1.65(9)	78(23)	17(2)	0.1266	652.881	37.012	5

Cu-S(2.2) Cu-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.20(1)	4(1)					
1S	2.30(2)	3(2)	neg2(1)	0.0375	193.606	10.976	5
2S	2.22(6)	16(4)					
2S	2.23(1)	5(1)	neg3(2)	0.0411	211.848	12.010	5
3S	2.23(1)	6(1)					
1S	2.15(8)	18(15)	neg4(2)	0.0387	199.580	11.314	5
4S	2.22(1)	8(1)					
1S	2.03(4)	18(7)	neg5(1)	0.0415	213.941	12.128	5
3S	2.23(1)	6(0)					
2S	2.49(0.31)	76(158)	neg1(3)	0.0399	205.869	11.671	5
5S	2.24(1)	10(1)					
1S	2.55(3)	10(4)	neg1(2)	0.0582	299.884	17.001	5
4S	2.24(1)	1(0)					
2S	2.62(8)	31(12)	neg2(2)	0.0384	198.163	11.234	5
3S	2.23(1)	6(0)					
3S	2.51(0.24)	80(117)	neg1(2)	0.0397	204.782	11.609	5
6S	2.23(1)	13(1)					
1S	1.20(0.13)	41(30)	neg3(2)	0.1123	579.157	32.833	5
5S	2.24(1)	10(1)					
2S	2.59(4)	20(6)	neg2(2)	0.0545	281.001	15.930	5
4S	2.23(1)	8(0)					
3S	1.98(0.11)	62(21)	neg3(2)	0.0428	220.654	12.509	5

Cu-N(2.0) Cu-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	2(1)					5
1S	2.30(1)	2(1)	10(1)	0.0427	220.391	12.494	
1N/O	2.05(2)	2(1)					5
2S	2.26(1)	5(1)	4(2)	0.0448	230.908	13.090	
2N/O	2.09(2)	5(2)					
2S	2.27(1)	6(1)	7(2)	0.0398	204.971	11.620	5
3N/O	2.10(1)	5(1)					
1S	2.29(1)	4(1)	11(1)	0.0454	234.201	13.277	5
1N/O	2.05(0.10)	20(20)					
3S	2.24(1)	7(1)	neg1(2)	0.0383	197.261	11.183	5
1N/O	2.33(0.20)	7(12)					
4S	2.24(1)	8(2)	neg2(2)	0.0392	201.884	11.445	5
4N/O	2.12(2)	8(2)					
1S	2.27(1)	4(1)	11(2)	0.0620	319.641	18.121	5
2N/O	2.09(8)	31(26)					
3S	2.24(1)	7(1)	0(2)	0.0389	200.619	11.373	5
3N/O	2.12(1)	6(2)					
2S	2.27(1)	8(2)	9(1)	0.0389	200.571	11.370	5
5N/O	2.12(3)	12(2)					
1S	2.26(1)	3(1)	11(2)	0.0872	449.556	25.486	5
1N/O	2.95(3)	1(3)					
5S	2.23(1)	11(1)	neg2(1)	0.0657	338.729	19.203	5
4N/O	2.14(1)	9(4)					
2S	2.26(1)	7(2)	10(2)	0.0440	226.899	12.863	5
2N/O	2.37(6)	9(10)					
4S	2.23(1)	8(1)	neg4(2)	0.0384	197.748	11.210	5
3N/O	2.10(0.12)	55(40)					
3S	2.24(1)	6(0)	neg1(2)	0.0395	203.776	11.552	5
6N/O	2.12(3)	16(3)					
1S	2.26(1)	2(1)	10(2)	0.1162	599.243	33.971	5
1N/O	2.38(2)	1(2)					
6S	2.25(1)	13(1)	neg3(2)	0.0778	401.020	22.734	5
5N/O	2.16(2)	14(4)	10(2)	0.0549	283.055	16.047	5

2S	2.26(1)	6(1)					
2N/O	2.36(3)	4(2)					
5S	2.25(1)	10(1)	neg3(2)	0.0439	226.282	12.828	5
4N/O	2.10(0.17)	75(53)					
3S	2.24(1)	6(0)	neg1(2)	0.0397	204.867	11.614	5
3N/O	2.38(3)	10(8)					
4S	2.23(1)	9(1)	neg5(2)	0.0387	199.513	11.311	5

Cu-N(2.0) Cu-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.11(1)	1(1)					5
1Br	2.46(3)	10(3)	14(2)	0.1762	908.355	51.495	
1N/O	1.83(5)	5(5)					5
2Br	2.27(2)	7(1)	neg29(7)	0.2408	1241.768	70.396	
2N/O	1.84(5)	9(5)					
2Br	2.27(2)	7(1)	neg28(7)	0.2318	1195.395	67.768	5
3N/O	2.12(1)	3(1)					
1Br	2.46(3)	11(3)	14(2)	0.1231	634.800	35.987	5
1N/O	1.82(4)	4(4)					
3Br	2.27(2)	9(1)	neg29(5)	0.1754	904.204	51.260	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(1)	4(1)					
1Br	2.45(3)	12(3)	13(1)	0.1349	695.637	37.436	5
2N/O	1.82(4)	9(4)					
3Br	2.27(2)	9(1)	neg29(5)	0.1710	881.506	49.973	5
3N/O	2.12(1)	3(1)					
2Br	2.49(3)	17(4)	14(1)	0.1209	623.460	35.344	5
5N/O	2.11(1)	6(1)					
1Br	2.44(3)	11(3)	12(2)	0.1844	950.803	53.901	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.12(1)	4(1)					
2Br	2.48(3)	18(4)	13(1)	0.1357	699.848	39.675	5

2N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
3N/O	1.82(5)	13(5)					
3Br	2.27(2)	9(1)	neg28(6)	0.1702	877.396	49.740	5
6N/O	2.10(2)	9(2)					
1Br	2.42(3)	10(3)	11(2)	0.2491	1284.586	72.824	5
1N/O	2.30(4)	1(3)					
6Br	2.29(2)	14(1)	neg27(4)	0.1098	566.080	32.091	5
5N/O	2.11(1)	6(1)					
2Br	2.46(4)	17(5)	12(1)	0.1883	971.134	55.054	5
2N/O	1.80(4)	10(4)					
5Br	2.27(2)	12(1)	neg29(4)	0.1180	608.236	34.481	5
4N/O	1.81(5)	16(6)					
3Br	2.27(2)	9(1)	neg28(6)	0.1700	876.378	49.682	5
3N/O	1.80(4)	14(5)					
4Br	2.27(2)	11(1)	neg29(5)	0.1376	709.642	40.230	5

Cu-N(2.0) Cu-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.09(3)	2(3)					
1Imd	2.15(2)	9(3)	11(2)	0.2609	1244.731	70.564	5
4N/O	2.10(2)	5(2)					
1Imd	1.69(7)	20(13)					
1Imd	2.17(4)	2(3)	13(2)	0.1572	810.411	51.818	7
3N/O	2.10(2)	2(1)					
1Imd	1.97(6)	8(9)					
1Imd	2.18(3)	1(2)					
1Imd	1.66(5)	13(8)	13(2)	0.1274	657.137	48.178	9
2N/O	2.11(2)	0(1)					
1Imd	1.90(6)	5(9)					
1Imd	2.18(3)	2(2)					
1Imd	2.04(4)	1(4)					
1Imd	1.64(5)	10(7)	12(2)	0.1265	652.325	56.043	11
1N/O	2.10(3)	2(2)					
1Imd	1.84(9)	3(20)					
1Imd	1.96(5)	5(12)					
1Imd	1.61(8)	10(12)					
1Imd	2.19(4)	6(6)	10(3)	0.1784	919.754	95.414	13

1Imd	2.07(4)	7(9)					
4N/O	2.10(2)	5(2)					
1Imd	2.17(4)	3(3)	13(2)	0.2012	1037.360	58.808	5
3N/O	2.11(2)	3(2)					
1Imd	1.67(6)	21(12)					
1Imd	2.18(3)	2(3)	15(2)	0.1370	706.382	45.166	7
2N/O	2.11(1)	0(1)					
1Imd	2.02(3)	2(3)					
1Imd	1.68(7)	19(12)					
1Imd	2.19(3)	0(2)	14(2)	0.1312	676.429	49.593	9
1N/O	2.11(2)	2(2)					
1Imd	1.66(8)	14(12)					
1Imd	2.18(3)	4(3)					
1Imd	2.06(4)	4(4)					
1Imd	1.95(6)	2(9)	12(2)	0.1730	892.273	76.658	11
0N/O							
1Imd	2.08(3)	11(4)					
1Imd	1.98(4)	10(5)					
1Imd	1.65(0.12)	12(17)					
1Imd	1.88(7)	3(9)					
1Imd	2.19(3)	10(4)	7(3)	0.3134	1615.975	138.834	11
3N/O	2.12(1)	3(1)					
1Imd	2.13(0.10)	10(11)	14(2)	0.1664	857.820	48.630	5
2N/O	2.11(2)	1(1)					
1Imd	2.20(3)	1(2)					
1Imd	1.65(4)	15(8)	17(2)	0.1380	658.384	42.097	7
1N/O	2.12(2)	2(2)					
1Imd	2.19(2)	2(2)					
1Imd	2.05(3)	1(2)					
1Imd	1.65(9)	23(17)	16(2)	0.1773	913.947	67.007	9
0N/O							
1Imd	2.07(3)	7(3)					
1Imd	2.19(2)	7(2)					
1Imd	1.67(0.16)	25(30)					
1Imd	1.97(4)	3(5)	11(3)	0.3283	1692.996	124.123	9
2N/O	2.12(2)	1(2)					
1Imd	2.15(6)	5(6)	16(2)	0.1831	944.179	53.526	5
1N/O							
1Imd			No Fit	No Fit	No Fit	No Fit	7

1Imd							
0N/O							
1Imd	1.97(3)	3(5)					
1Imd	2.07(3)	7(3)					
1Imd	2.19(2)	7(2)	10(2)	0.3473	1790.766	114.502	7

Cu-N(2.0) Cu-S(2.2) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	1(1)					
1Imd	2.07(5)	8(5)	8(2)	0.0466	240.200	15.358	7
0N/O							
1S	2.26(1)	2(1)					
1Imd	2.02(0.14)	9(15)					
1Imd	2.05(5)	2(4)	4(3)	0.1092	562.825	35.987	7

Cu-N(2.0) Cu-S(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	2(1)					
1Imd	2.06(5)	8(5)	8(2)	0.0469	241.901	15.467	7
0N/O							
1S	2.26(1)	2(1)					
1Imd	2.05(5)	2(3)					
1Imd	2.01(0.12)	9(15)	3(3)	0.1057	545.200	34.860	7

Cu-N(2.0) Cu-S(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	2(1)					
1Imd	2.07(5)	7(4)	7(2)	0.0423	217.857	13.930	7
0N/O							
1S	2.27(1)	2(1)					
1Imd	2.03(3)	1(3)					
1Imd	2.14(5)	2(7)	5(2)	0.0889	458.177	29.296	7

Cu-N(2.0) Cu-S(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(3)	1(3)					
1S	3.04(0.26)	26(49)	16(0)	0.2788	1437.711	91.927	7

1Imd	2.14(5)	3(5)					
0N/O							
1S	2.44(3)	0(2)					
1Imd	1.29(5)	4(5)					
1Imd	2.23(5)	0(3)	neg48(8)	0.3118	1607.625	102.792	7

Cu-N(2.0) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(3)	1(3)					
1S	3.07(0.27)	27(53)					
1Imd	2.14(6)	3(5)	16(4)	0.2798	1442.598	92.240	7
0N/O							
1S	3.10(3)	1(3)					
1Imd	2.18(1)	5(2)					
1Imd	2.06(1)	4(2)	14(0)	0.3206	1653.203	105.706	7

Cu-N(2.0) Cu-S(2.2) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.25(1)	5(0)					
2Imd	2.03(2)	4(2)	neg1(1)	0.0339	174.685	9.903	5

Cu-N(2.0) Cu-S(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.25(1)	4(0)					
2Imd	2.02(2)	4(2)	0(1)	0.0383	197.536	11.198	5

Cu-N(2.0) Cu-S(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.25(1)	4(0)					
2Imd	2.02(2)	4(2)	neg1(1)	0.0367	189.180	10.725	5

Cu-N(2.0) Cu-S(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.24(1)	5(0)					
2Imd	2.01(2)	5(2)	neg1(1)	0.0356	183.504	10.403	5

Cu-N(2.0) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
0N/O							
1S	2.42(2)	3(1)					
2Imd	1.75(6)	6(5)	neg51(6)	0.2698	1390.951	78.854	5

Cu-N(2.0) Cu-S(2.2) Cu-S(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.96(3)	5(3)					
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
0Imd			0(2)	0.0297	152.916	9.777	7
0N/O							
1S	2.19(1)	0(1)					
1S	2.30(1)	0(1)					
1Imd	1.99(2)	6(2)	0(1)	0.0235	121.417	7.763	7

Cu-N(2.0) Cu-S(2.2) Cu-S(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	5(3)					
1S	2.19(1)	1(1)					
1S	2.30(1)	0(1)					
0Imd			neg1(2)	0.0293	151.182	9.667	7
0N/O							
1S	2.19(1)	0(1)					
1S	2.30(1)	0(1)					
1Imd	1.99(2)	6(2)	0(1)	0.0227	116.801	7.468	7

Cu-N(2.0) Cu-S(2.2) Cu-S(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	6(3)					
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
0Imd			neg1(2)	0.0290	149.609	9.566	7
0N/O							
1S	2.19(1)	0(1)					
1S	2.30(1)	0(1)					
1Imd	1.99(2)	6(2)	neg1(1)	0.2210	114.077	7.294	7

Cu-N(2.0) Cu-S(2.2) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	2.06(1)	2(1)					
1S	2.28(1)	1(1)					
1S	2.84(7)	15(9)					
0Imd			7(3)	0.0779	401.515	25.673	7
0N/O							
1S	2.26(1)	1(1)					
1S	2.93(0.15)	22(25)					
1Imd	2.03(2)	1(2)	3(3)	0.1247	642.727	41.096	7

Cu-N(2.0) Cu-S(2.3) Cu-S(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	5(3)					
1S	2.30(1)	1(1)					
1S	2.19(1)	1(1)					
0Imd			neg1(2)	0.0294	151.529	9.689	7
0N/O							
1S	2.19(1)	0(1)					
1S	2.30(1)	0(1)					
1Imd	1.98(2)	6(2)	neg1(1)	0.0218	112.633	7.202	7

Cu-N(2.0) Cu-S(2.3) Cu-S(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	5(3)					
1S	2.18(1)	1(1)					
1S	2.30(1)	1(1)					
0Imd			neg2(2)	0.0284	146.387	9.360	7
0N/O							
1S	2.19(1)	0(1)					
1S	2.30(1)	0(1)					
1Imd	2.00(2)	6(2)	neg1(1)	0.0206	106.133	6.786	7

Cu-N(2.0) Cu-S(2.3) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	6(3)					
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
0Imd			neg2(2)	0.0282	145.641	9.312	7
0N/O							
1S	2.26(1)	1(1)					
1S	2.93(0.15)	23(26)					
1Imd	2.03(2)	1(2)	3(3)	0.1229	633.497	40.506	7

Cu-N(2.0) Cu-S(2.4) Cu-S(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.95(3)	5(3)					
1S	2.30(1)	1(1)					
1S	2.19(1)	1(1)					
0Imd			neg2(2)	0.0291	150.298	9.610	7
0N/O							
1S	2.30(1)	0(1)					
1S	2.19(1)	1(1)					
1Imd	1.98(2)	6(2)	neg2(1)	0.0215	111.010	7.098	7

Cu-N(2.0) Cu-S(2.4) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(1)	2(1)					
1S	2.29(1)	1(1)					
1S	3.73(7)	10(9)					
0Imd			7(2)	0.0754	388.716	24.854	7
0N/O							
1S	2.26(1)	1(1)					
1S	3.83(0.19)	16(29)					
1Imd	2.03(2)	1(1)	3(3)	0.1226	632.330	40.431	7

Cu-N(2.0) Cu-S(2.5) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	1(1)					
1S	2.83(7)	14(9)					
1S	2.28(1)	1(1)					
0Imd			5(3)	0.0867	446.857	28.572	7
0N/O							
1S	2.91(0.16)	23(27)					
1S	2.25(1)	1(1)					
1Imd	2.03(2)	1(2)	1(3)	0.1181	608.739	38.923	7

Cu-N(2.0) Cu-S(2.2) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	2(1)					
1S	2.30(1)	3(1)					
1Imd	2.20(7)	13(11)	11(1)	0.0371	177.014	11.318	7
1N/O	2.08(1)	1(1)					
1S	2.29(1)	1(1)					
1Imd	2.21(5)	5(5)					
1Imd	2.02(4)	5(4)	10(2)	0.0442	227.659	16.691	9

Cu-N(2.0) Cu-S(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(1)	2(1)					
1S	2.30(1)	3(1)					
1Imd	2.19(6)	13(10)	11(1)	0.0359	185.174	11.840	7
1N/O	2.08(1)	1(1)					
1S	2.29(1)	2(1)					
1Imd	2.20(4)	5(5)					
1Imd	2.02(4)	5(3)	9(2)	0.0436	224.678	16.472	9

Cu-N(2.0) Cu-S(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	2(1)					
1S	2.29(1)	3(1)					
1Imd	2.18(6)	11(8)	10(1)	0.0331	170.880	10.926	7
1N/O	2.07(1)	1(1)					
1S	2.29(1)	2(1)					
1Imd	2.02(3)	4(3)					
1Imd	2.20(4)	4(4)	8(2)	0.0314	161.992	11.877	9

Cu-N(2.0) Cu-S(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.12(2)	1(2)					
1S	2.99(0.18)	24(34)					
1Imd	2.13(7)	5(7)	15(2)	0.1727	890.536	56.941	7
1N/O	2.12(2)	2(2)					
1S	3.03(0.15)	18(25)					
1Imd	2.04(3)	2(2)					
1Imd	2.18(2)	2(2)	14(2)	0.1858	957.774	70.220	9

Cu-N(2.0) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.12(2)	1(2)					
1S	3.01(0.20)	26(39)					
1Imd	2.13(7)	5(7)	16(2)	0.1733	893.814	57.150	7
1N/O	2.12(2)	2(2)					
1S	3.05(0.14)	18(24)					
1Imd	2.18(2)	2(2)					
1Imd	2.04(3)	2(2)	14(2)	0.1860	958.796	70.295	9

Cu-N(2.0) Cu-S(2.2) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.97(8)	14(10)					
2S	2.25(1)	5(1)					
1Imd	2.05(3)	4(2)	2(2)	0.0321	165.644	10.591	7
0N/O							
2S	2.25(1)	5(1)					
1Imd	2.01(0.14)	19(20)					
1Imd	2.04(4)	5(3)	1(2)	0.0382	196.897	12.590	7

Cu-N(2.0) Cu-S(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.00(9)	15(11)					
2S	2.25(1)	5(1)					
1Imd	2.06(3)	4(2)	1(2)	0.0300	154.657	9.889	7
0N/O							
2S	2.25(1)	5(1)					
1Imd	2.06(6)	6(6)					
1Imd	2.06(0.14)	13(16)	1(2)	0.0311	160.590	10.268	7

Cu-N(2.0) Cu-S(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(3)	3(2)					
2S	2.26(1)	6(1)					
1Imd	2.03(5)	10(6)	3(2)	0.0334	172.040	11.000	7
0N/O							
2S	2.25(1)	5(1)					
1Imd	2.04(5)	5(3)					
1Imd	1.98(0.10)	16(17)	0(2)	0.0334	172.395	11.023	7

Cu-N(2.0) Cu-S(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(3)	3(2)					
2S	2.26(1)	6(1)					
1Imd	2.02(5)	10(6)	2(2)	0.0335	172.947	11.058	7
0N/O							
2S	3.09(5)	9(6)					
1Imd	2.18(2)	5(2)					
1Imd	2.06(2)	4(2)	15(3)	0.3505	1807.285	115.558	7

Cu-N(2.0) Cu-S(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(3)	1(3)					
2S	3.04(0.18)	33(38)					
1Imd	2.13(5)	3(5)	15(0)	0.2771	1428.838	91.360	7
0N/O							
2S	3.09(4)	9(6)					
1Imd	2.18(1)	5(2)					
1Imd	2.06(1)	4(2)	14(0)	0.3490	1799.352	115.051	7

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(2)	2(2)					
1S	2.24(2)	0(2)					
1S	2.15(2)	1(3)					
1Imd	1.91(2)	1(2)	neg4(2)	0.0472	840.750	61.640	9
0N/O							
1S	2.22(2)	0(1)					
1S	2.16(4)	7(7)					
1Imd	1.99(3)	1(4)					
1Imd	1.86(2)	0(2)	neg2(2)	0.0464	825.868	60.549	9

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.93(5)	11(6)					
1S	2.19(1)	0(1)					
1S	2.30(1)	0(1)					
1Imd	2.04(4)	8(40	0(2)	0.0210	108.163	7.930	9
0N/O							
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Imd	2.13(4)	7(6)					
1Imd	1.97(3)	5(3)	1(1)	0.0218	112.197	8.226	9

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(4)	1(2)					
1S	2.29(5)	2(2)					
1S	2.19(4)	8(18)					
1Imd	2.01(4)	7(4)	3(2)	0.0325	167.642	12.291	9
0N/O							
1S	2.19(1)	0(1)	0(1)	0.0213	109.889	8.057	9

1S	2.30(1)	0(1)					
1Imd	1.96(3)	5(3)					
1Imd	2.13(4)	7(6)					

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	1(1)					
1S	2.29(1)	1(1)					
1S	2.89(7)	17(11)					
1Imd	2.02(5)	6(4)	7(2)	0.0426	219.536	16.095	9
0N/O							
1S	2.26(1)	2(1)					
1S	2.94(0.13)	20(21)					
1Imd	2.05(6)	2(4)					
1Imd	2.01(0.14)	8(15)	3(3)	0.1002	516.664	37.880	9

Cu-N(2.0) Cu-S(2.3) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(4)	2(2)					
1S	2.16(3)	4(10)					
1S	2.29(2)	0(2)					
1Imd	2.00(3)	6(3)	1(2)	0.0291	150.027	10.999	9
0N/O							
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Imd	2.12(4)	7(6)					
1Imd	1.96(2)	5(3)	0(1)	0.0208	107.033	7.847	9

Cu-N(2.0) Cu-S(2.3) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(4)	1(1)					
1S	2.29(4)	1(2)					
1S	2.18(4)	7(15)					
1Imd	2.00(3)	6(4)	2(2)	0.0314	162.035	11.880	9
0N/O							
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Imd	1.96(2)	5(3)					
1Imd	2.12(4)	7(6)	0(1)	0.0203	104.849	7.687	9

Cu-N(2.0) Cu-S(2.3) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	1(1)					
1S	2.28(1)	1(10					
1S	2.88(7)	16(10)					
1Imd	2.01(4)	6(4)	6(2)	0.0431	222.238	16.294	9
0N/O							
1S	2.26(1)	1(1)					
1S	2.94(0.14)	20(21)					
1Imd	2.05(5)	2(3)					
1Imd	2.00(0.11)	8(14)	3(3)	0.0974	502.255	36.823	9

Cu-N(2.0) Cu-S(2.4) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(4)	2(2)					
1S	2.16(3)	5(10)					
1S	2.29(2)	1(2)					
1Imd	2.01(3)	5(3)	1(2)	0.0261	134.630	9.871	9
0N/O							
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Imd	2.13(3)	5(4)					
1Imd	1.98(2)	4(2)	0(1)	0.0171	88.208	6.467	9

Cu-N(2.0) Cu-S(2.4) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	2(1)					
1S	2.28(1)	1(1)					
1S	2.87(6)	16(9)					
1Imd	2.00(4)	5(3)	5(2)	0.0434	223.871	16.413	9
0N/O							
1S	2.26(1)	1(1)					
1S	2.93(0.14)	21(22)					
1Imd	2.05(5)	1(3)					
1Imd	1.98(0.10)	8(13)	2(3)	0.0948	488.751	35.833	9

Cu-N(2.0) Cu-S(2.5) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	2(1)					
1S	2.86(6)	14(8)					
1S	2.28(1)	1(1)					
1Imd	1.98(4)	5(3)	4(2)	0.0439	226.509	16.607	9

0N/O							
1S	3.11(3)	2(3)					
1S	1.80(4)	17(7)					
1Imd	2.08(1)	4(2)					
1Imd	2.19(1)	5(2)	16(0)	0.2297	1184.602	86.850	9

Cu-S(2.2) Cu-S(2.3) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.16(2)	4(1)					
1S	2.27(2)	4(1)					
1Br	2.15(2)	2(2)					
1Imd	2.01(2)	3(1)	neg1(1)	0.0191	98.405	7.215	9

Cu-S(2.2) Cu-S(2.3) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.56(4)	18(5)					
1Imd	1.98(2)	6(2)	0(1)	0.0199	102.659	7.527	9

Cu-S(2.2) Cu-S(2.3) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.57(4)	18(5)					
1Imd	1.98(2)	6(2)	0(1)	0.0200	102.983	7.550	9

Cu-S(2.2) Cu-S(2.3) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.57(4)	18(5)					
1Imd	1.98(2)	6(2)	0(1)	0.0200	103.306	7.574	9

Cu-S(2.2) Cu-S(2.4) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.16(1)	5(1)					
1S	2.27(1)	4(1)					
1Br	2.15(2)	1(1)					
1Imd	2.02(2)	3(1)	neg1(1)	0.0160	82.395	6.041	9

Cu-S(2.2) Cu-S(2.4) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Br	1.87(3)	21(5)					
1Imd	2.02(3)	7(3)	neg1(1)	0.0184	94.968	6.963	9

Cu-S(2.2) Cu-S(2.4) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(5)	18(5)					
1Imd	1.98(2)	6(2)	neg1(1)	0.0195	100.637	7.378	9

Cu-S(2.2) Cu-S(2.4) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(5)	18(5)					
1Imd	1.98(2)	6(2)	neg1(1)	0.0195	100.802	7.390	9

Cu-S(2.2) Cu-S(2.5) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.56(5)	18(5)					
1Imd	1.98(2)	7(3)	neg1(1)	0.0193	99.394	7.287	9

Cu-S(2.2) Cu-S(2.5) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Br	1.86(3)	21(4)					
1Imd	2.02(3)	7(3)	neg1(1)	0.0181	93.467	6.853	9

Cu-S(2.2) Cu-S(2.5) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(5)	18(5)					
1Imd	1.97(2)	6(3)	neg1(1)	0.0193	99.275	7.278	9

Cu-S(2.2) Cu-S(2.5) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(5)	18(5)					
1Imd	1.97(2)	6(3)	neg1(1)	0.0193	99.323	7.282	9

Cu-S(2.2) Cu-S(2.6) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	0(1)					
1S	2.79(2)	4(2)					
1Br	2.38(1)	5(1)					
1Imd	1.92(3)	4(2)	neg8(2)	0.0477	245.778	18.019	9

Cu-S(2.2) Cu-S(2.6) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	0(1)					
1S	2.30(1)	0(1)					
1Br	2.56(5)	18(5)					
1Imd	1.97(2)	7(3)	neg1(1)	0.0190	98.213	7.201	9

Cu-S(2.2) Cu-S(2.6) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	0(1)					
1S	2.30(1)	0(1)					
1Br	2.57(5)	18(5)					
1Imd	1.97(2)	7(3)	neg1(1)	0.0191	98.226	7.202	9

Cu-S(2.2) Cu-S(2.6) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	0(1)					
1S	2.80(2)	4(1)					
1Br	2.75(2)	0(1)					
1Imd	2.00(3)	1(2)	neg1(3)	0.0793	408.680	29.963	9

Cu-S(2.3) Cu-S(2.4) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.17(1)	6(1)					
1S	2.28(1)	5(1)					
1Br	2.16(2)	1(1)					
1Imd	2.03(2)	4(2)	neg1(1)	0.0148	76.250	5.590	9

Cu-S(2.3) Cu-S(2.4) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.56(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0186	95.662	7.013	9

Cu-S(2.3) Cu-S(2.4) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0186	95.874	7.029	9

Cu-S(2.3) Cu-S(2.4) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0186	96.053	7.042	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.56(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0183	94.564	6.933	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Br	1.86(4)	22(5)					
1Imd	2.01(3)	7(3)	neg1(1)	0.0177	91.372	6.699	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0183	94.539	6.931	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0183	94.610	6.936	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	0(1)					
1S	2.79(2)	4(2)					
1Br	2.38(1)	5(1)					
1Imd	1.92(2)	4(2)	neg9(2)	0.0443	228.497	16.752	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(5)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0181	93.449	6.851	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0181	93.507	6.856	9

Cu-S(2.3) Cu-S(2.5) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	0(1)					
1S	2.80(2)	4(1)					
1Br	2.75(2)	0(1)					
1Imd	2.00(3)	1(2)	neg2(3)	0.0760	391.940	28.735	9

Cu-S(2.3) Cu-S(2.6) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.56(4)	18(5)					
1Imd	1.97(2)	6(2)	neg1(1)	0.0180	92.885	6.810	9

Cu-S(2.3) Cu-S(2.6) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.19(1)	0(1)					
1S	2.31(1)	0(1)					
1Br	1.86(4)	22(5)					
1Imd	2.01(3)	7(3)	neg2(1)	0.0177	91.488	6.708	9

Cu-S(2.3) Cu-S(2.6) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	3.13(4)	3(4)					
1S	1.92(3)	9(3)					
1Br	2.59(0.11)	19(15)					
1Imd	2.17(2)	0(2)	27(3)	0.2504	1291.019	94.652	9

Cu-S(2.3) Cu-S(2.6) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	1(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg2(1)	0.0180	93.016	6.819	9

Cu-S(2.4) Cu-S(2.5) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	0(1)					
1S	2.79(2)	4(2)					
1Br	2.38(1)	5(1)					
1Imd	1.91(2)	4(2)	neg9(2)	0.0420	216.785	15.894	9

Cu-S(2.4) Cu-S(2.5) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg2(1)	0.0178	91.837	6.733	9

Cu-S(2.4) Cu-S(2.5) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.30(1)	0(1)					
1Br	2.57(4)	18(5)					
1Imd	1.97(2)	6(2)	neg2(1)	0.0178	91.925	6.740	9

Cu-S(2.4) Cu-S(2.5) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	1.99(1)	2(1)					
1S	1.84(3)	8(3)					
1Br	3.11(0.12)	18(17)					
1Imd	1.99(9)	19(24)	31(2)	0.1506	776.285	56.914	9

Cu-S(2.4) Cu-S(2.6) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.78(2)	4(2)					
1Br	2.38(1)	5(1)					
1Imd	1.91(2)	4(2)	neg9(2)	0.0404	208.110	15.258	9

Cu-S(2.4) Cu-S(2.6) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.30(1)	0(1)					
1S	2.19(1)	0(1)					
1Br	1.86(4)	23(5)					
1Imd	2.00(3)	6(3)	neg2(1)	0.0183	94.105	6.899	9

Cu-S(2.4) Cu-S(2.6) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.18(1)	1(1)					
1S	2.78(2)	4(2)					
1Br	2.38(1)	5(1)					
1Imd	1.91(2)	4(2)	neg9(2)	0.0431	222.394	16.305	9

Cu-S(2.4) Cu-S(2.6) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	3.05(3)	1(3)					
1S	2.27(1)	1(1)					
1Br	3.02(4)	5(5)					
1Imd	2.04(2)	0(1)	3(3)	0.1046	539.225	39.534	9

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.57(5)	18(7)					
1Imd	2.06(6)	10(7)	8(2)	0.0412	196.446	14.403	9
0N/O			0(4)	0.0871	448.861	32.909	9

1S	2.23(2)	1(1)					
1Br	2.43(3)	10(3)					
1Imd	1.96(0.15)	14(21)					
1Imd	2.03(5)	3(4)					

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.57(6)	18(7)					
1Imd	2.06(6)	10(7)	8(2)	0.0417	215.230	15.780	9
0N/O							
1S	2.23(2)	2(1)					
1Br	2.43(4)	11(4)					
1Imd	1.96(0.15)	13(21)					
1Imd	2.03(5)	3(3)	0(4)	0.0898	462.918	33.939	9

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.58(6)	18(7)					
1Imd	2.06(6)	10(7)	8(2)	0.0422	217.450	15.942	9
0N/O							
1S	2.24(2)	2(1)					
1Br	2.44(4)	11(4)					
1Imd	2.03(5)	3(3)					
1Imd	1.96(0.15)	13(20)	0(4)	0.0921	474.707	34.803	9

Cu-N(2.0) Cu-S(2.2) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.58(6)	18(7)					
1Imd	2.06(7)	10(7)	8(2)	0.0426	219.583	16.099	9
0N/O							
1S	2.24(2)	2(1)					
1Br	2.44(4)	12(4)					
1Imd	2.03(5)	3(3)					
1Imd	1.96(0.15)	13(20)	0(4)	0.0940	484.803	35.544	9

Cu-N(2.0) Cu-S(2.3) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(1)	2(1)					
1S	2.30(1)	1(1)					
1Br	1.92(2)	16(3)					
1Imd	2.10(5)	9(6)	8(2)	0.0293	151.045	11.074	9
0N/O							
1S	2.23(2)	2(1)					
1Br	2.43(3)	10(3)					
1Imd	1.95(0.14)	13(19)					
1Imd	2.02(5)	3(3)	neg1(4)	0.0840	433.291	31.767	9

Cu-N(2.0) Cu-S(2.3) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.57(6)	18(7)					
1Imd	2.05(6)	9(6)	8(2)	0.0424	218.603	16.027	9
0N/O							
1S	2.23(2)	2(1)					
1Br	2.43(4)	11(4)					
1Imd	2.03(5)	3(3)					
1Imd	1.95(0.13)	13(19)	neg1(4)	0.0866	446.744	32.753	9

Cu-N(2.0) Cu-S(2.3) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.58(6)	18(7)					
1Imd	2.05(6)	9(6)	8(2)	0.0429	221.085	16.209	9
0N/O							
1S	2.24(2)	2(1)					
1Br	2.44(4)	12(4)					
1Imd	2.03(5)	3(3)					
1Imd	1.95(0.13)	13(19)	neg1(4)	0.0888	457.950	33.575	9

Cu-N(2.0) Cu-S(2.3) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.58(6)	18(7)					
1Imd	2.05(6)	9(6)	8(2)	0.0433	223.457	16.383	9

0N/O							
1S	2.24(2)	2(1)					
1Br	2.44(4)	12(4)					
1Imd	2.03(5)	2(3)					
1Imd	1.96(0.13)	12(18)	0(4)	0.0907	467.483	34.274	9

Cu-N(2.0) Cu-S(2.4) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(1)	2(1)					
1S	2.30(1)	1(1)					
1Br	1.91(3)	16(3)					
1Imd	2.09(5)	9(6)	8(2)	0.0301	155.129	11.373	9
0N/O							
1S	2.23(2)	2(1)					
1Br	2.43(3)	10(4)					
1Imd	2.02(5)	3(3)					
1Imd	1.94(0.13)	13(18)	neg2(4)	0.0814	419.475	30.754	9

Cu-N(2.0) Cu-S(2.4) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.57(6)	18(7)					
1Imd	2.03(5)	8(5)	7(2)	0.0428	220.665	16.178	9
0N/O							
1S	2.24(2)	2(1)					
1Br	2.43(4)	11(4)					
1Imd	2.03(5)	3(3)					
1Imd	1.94(0.12)	12(17)	neg1(4)	0.0838	432.203	31.687	9

Cu-N(2.0) Cu-S(2.4) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.58(6)	18(7)					
1Imd	2.03(5)	8(5)	7(2)	0.0433	223.306	16.372	9
0N/O							
1S	2.24(2)	2(1)					
1Br	2.44(4)	12(4)					
1Imd	2.03(4)	2(3)					
1Imd	1.94(0.12)	12(17)	neg1(4)	0.0859	442.892	32.471	9

Cu-N(2.0) Cu-S(2.4) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(2)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.58(6)	18(8)					
1Imd	2.03(5)	8(6)	7(2)	0.0438	225.842	16.558	9
0N/O							
1S	2.24(2)	2(1)					
1Br	2.44(4)	12(5)					
1Imd	2.03(4)	2(3)					
1Imd	1.95(0.12)	12(17)	neg1(4)	0.0877	452.022	33.140	9

Cu-N(2.0) Cu-S(2.5) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	1(1)					
1S	2.29(1)	1(1)					
1Br	2.57(6)	18(7)					
1Imd	2.03(5)	8(5)	6(2)	0.0428	220.661	16.178	9
0N/O							
1S	2.23(2)	2(1)					
1Br	2.42(3)	10(4)					
1Imd	2.02(5)	3(3)					
1Imd	1.93(0.12)	13(17)	neg2(4)	0.0792	408.512	29.950	9

Cu-N(2.0) Cu-S(2.5) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	1(1)					
1S	2.28(1)	1(1)					
1Br	2.57(6)	18(7)					
1Imd	2.02(5)	8(5)	6(2)	0.0433	223.428	16.381	9
0N/O							
1S	2.23(2)	2(1)					
1Br	2.43(4)	11(4)					
1Imd	2.02(4)	2(3)					
1Imd	1.94(0.11)	12(16)	neg2(4)	0.0816	420.813	30.852	9

Cu-N(2.0) Cu-S(2.5) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(2)	1(2)					
1S	2.86(4)	6(5)					
1Br	2.43(2)	7(2)					
1Imd	2.09(8)	5(7)	12(4)	0.1995	1028.616	75.414	9

0N/O							
1S	2.24(2)	2(1)					
1Br	2.43(4)	12(4)					
1Imd	1.94(0.11)	12(16)					
1Imd	2.03(4)	2(3)	neg1(4)	0.0836	431.060	31.603	9

Cu-N(2.0) Cu-S(2.5) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(2)	1(2)					
1S	2.86(4)	5(4)					
1Br	2.44(2)	8(2)					
1Imd	2.09(7)	5(7)	12(3)	0.2015	1038.947	76.171	9
0N/O							
1S	3.01(0.12)	5(20)					
1Br	2.92(0.11)	6(7)					
1Imd	2.06(2)	4(2)					
1Imd	2.18(2)	5(2)	14(0)	0.3309	1706.212	125.092	9

Cu-N(2.0) Cu-S(2.6) Cu-Br(2.3) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(2)	1(2)					
1S	2.88(6)	8(8)					
1Br	2.43(2)	7(2)					
1Imd	2.07(7)	5(7)	11(4)	0.1971	1016.181	74.502	9
0N/O							
1S	2.52(2)	1(1)					
1Br	2.23(2)	4(1)					
1Imd	1.86(3)	2(3)					
1Imd	1.74(8)	8(11)	neg35(5)	0.1191	613.991	45.015	9

Cu-N(2.0) Cu-S(2.6) Cu-Br(2.4) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.112)	1(2)					
1S	2.90(7)	10(10)					
1Br	2.44(3)	7(2)					
1Imd	2.08(7)	4(7)	12(4)	0.2017	1040.102	76.256	9
0N/O							
1S	2.52(2)	1(1)					
1Br	2.23(2)	4(1)					
1Imd	1.85(3)	2(3)					
1Imd	1.74(8)	8(12)	neg35(5)	0.1192	614.590	45.059	9

Cu-N(2.0) Cu-S(2.6) Cu-Br(2.5) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(2)	1(2)					
1S	2.88(6)	8(7)					
1Br	2.44(3)	8(2)					
1Imd	2.09(8)	5(7)	12(4)	0.2049	1056.632	77.468	9
0N/O							
1S	3.09(3)	2(3)					
1Br	2.47(5)	11(5)					
1Imd	2.05(2)	4(2)					
1Imd	2.17(2)	4(2)	12(3)	0.2787	1437.172	105.367	9

Cu-N(2.0) Cu-S(2.6) Cu-Br(2.6) Cu-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.15(2)	4(2)					
1S	2.82(3)	5(3)					
1Br	2.77(3)	1(3)					
1Imd	2.06(4)	1(3)	14(3)	0.2527	1302.872	95.521	9
0N/O							
1S	2.88(4)	3(3)					
1Br	2.83(5)	1(4)					
1Imd	2.05(3)	4(3)					
1Imd	2.16(3)	4(2)	12(3)	0.3472	1790.344	131.260	9

Table J.4. Additional Fits for Ni(II) H21L-InrS in Buffer with 10 mM Hepes, 1 M NaBr, 5 mM TCEP at 8.1.
Data Fit from k = 2 - 14 Å^{-1} and r = 1- 4 Å.

Ni-N(2.0)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.12(1)	1(1)	21(3)	0.3595	5878.610	299.324	3
3N/O	2.11(1)	1(1)	18(2)	0.3666	6529.876	332.484	3
4N/O	2.10(2)	4(1)	16(2)	0.4156	7403.667	376.976	3
5N/O	2.08(3)	7(2)	13(3)	0.4654	8289.429	422.076	3
6N/O	2.06(3)	11(3)	11(3)	0.4998	8903.220	453.329	3
7N/O	2.04(4)	13(4)	9(3)	0.5276	9397.815	478.512	3

Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.22(1)	3(1)	3(3)	0.2317	4127.878	210.181	3
3S	2.21(2)	6(1)	1(3)	0.2437	4340.703	221.017	3

4S	2.20(2)	9(1)	0(3)	0.2742	4883.926	248.677	3
5S	2.20(2)	11(1)	neg2(3)	0.3049	5430.930	276.529	3
6S	2.19(3)	14(2)	neg3(3)	0.3326	5924.851	301.678	3
7S	2.18(3)	16(2)	neg4(4)	0.3579	6374.201	324.558	3

Ni-N(2.0) Ni-N(2.2)

	r(Å)	**σ^2(x10^{-3} Å^2)**	**ΔE_o(eV)**	**R factor**	**Reduced χ^2**	**χ^2**	**nvar**
2N/O	2.00(3)	3(3)					
1N/O	2.12(1)	4(1)	12(3)	0.2463	4386.491	248.672	5
2N/O	2.10(1)	2(1)					
2N/O	1.97(2)	2(2)	10(2)	0.2343	4173.532	236.599	5
3N/O	2.09(1)	0(1)					
1N/O	1.92(2)	2(2)	11(2)	0.2420	4309.964	244.334	5
4N/O	2.08(1)	2(1)					
1N/O	1.90(2)	2(1)	11(2)	0.2448	4360.862	247.219	5
3N/O	2.09(1)	0(1)					
2N/O	1.94(2)	1(2)	9(2)	0.2306	4108.186	232.895	5
5N/O	2.09(3)	7(2)					
1N/O	1.55(0.16)	33(45)	16(3)	0.4410	7854.932	445.300	5
4N/O	2.11(2)	3(1)					
2N/O	2.54(6)	9(10)	18(2)	0.3084	5492.901	311.395	5
3N/O	2.10(1)	0(1)					
3N/O	1.94(2)	4(2)	8(2)	0.2415	4302.517	243.912	5
6N/O	2.05(3)	11(3)					
1N/O	3.37(0.10)	0(9)	11(3)	0.4887	8704.608	493.468	5
5N/O	2.10(3)	6(2)					
2N/O	1.57(0.12)	49(40)	17(4)	0.4236	7544.927	427.725	5
4N/O	2.09(1)	1(1)					
3N/O	1.92(2)	3(2)	7(2)	0.2724	4851.536	275.036	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.19(1)	1(1)					
1S	2.04(2)	2(1)	neg6(3)	0.1238	2204.412	124.969	5
2S	2.20(1)	1(1)					
2S	2.05(1)	6(1)	neg9(2)	0.0993	1769.609	100.320	5

3S	2.18(1)	3(0)					
1S	2.01(1)	2(1)	neg7(2)	0.0978	1741.423	98.722	5
4S	2.21(2)	9(1)					
1S	1.65(0.12)	28(19)	1(4)	0.2623	4671.932	264.854	5
3S	2.19(1)	3(0)					
2S	2.02(1)	5(1)	neg9(2)	0.0947	1686.127	95.587	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.18(1)	4(1)					
2S	2.00(1)	4(1)	neg10(2)	0.1088	1938.586	109.899	5
3S	2.19(1)	3(1)					
3S	2.03(1)	7(1)	neg11(2)	0.1059	1886.271	106.934	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.17(1)	6(1)					
2S	1.99(1)	4(1)	neg10(2)	0.1361	2423.478	137.388	5
4S	2.18(1)	4(1)					
3S	2.01(1)	7(1)	neg11(2)	0.1296	2308.280	130.857	5

Ni-N(2.0) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.93(2)	5(2)					5
1S	2.21(1)	0(0)	2(2)	0.1145	2039.337	115.611	
1N/O	1.88(1)	0(1)					5
2S	2.20(1)	3(1)	neg1(2)	0.0958	1706.404	96.737	
2N/O	1.89(1)	4(1)					
2S	2.21(1)	3(0)	neg1(2)	0.0944	1680.738	95.282	5
3N/O	1.94(2)	8(2)					
1S	2.22(1)	0(0)	2(2)	0.1021	1819.358	103.140	5
1N/O	1.86(1)	0(1)					
3S	2.20(1)	6(1)	neg2(2)	0.1117	1990.071	112.818	5
1N/O	2.35(1)	3(1)					
4S	2.19(3)	11(2)	neg4(4)	0.1770	3153.662	178.783	5
4N/O	1.95(3)	11(2)					
1S	2.22(1)	0(1)	2(2)	0.1057	1882.543	106.722	5

2N/O	1.87(2)	3(1)					
3S	2.20(1)	5(1)	neg3(2)	0.1419	2527.026	143.258	5
3N/O	1.89(2)	7(2)					
2S	2.21(1)	3(1)	neg1(2)	0.1178	2097.580	118.913	5
5N/O	1.96(4)	15(3)					
1S	2.22(1)	0(1)	3(3)	0.1160	2066.488	117.150	5
1N/O	2.35(1)	3(1)					
5S	2.19(3)	14(2)	neg5(4)	0.1705	3036.415	172.136	5
4N/O	1.90(3)	11(3)					
2S	2.21(1)	3(1)	neg1(2)	0.1468	2614.754	148.232	5
2N/O	2.12(0.30)	37(149)					
4S	2.21(3)	9(2)	1(8)	0.2663	4742.949	268.880	5
3N/O	2.06(0.15)	32(39)					
3S	2.22(2)	6(1)	3(6)	0.2200	3918.676	222.152	5
6N/O	1.98(5)	19(4)					
1S	2.22(1)	0(1)	4(4)	0.1275	2270.331	128.706	5
1N/O	2.35(1)	3(1)					
6S	2.18(3)	16(2)	neg6(4)	0.1702	3032.103	171.891	5
5N/O	2.09(0.10)	28(16)					
2S	2.23(2)	4(1)	8(6)	0.1600	2849.227	161.524	5
2N/O	2.10(1)	1(1)					
5S	2.14(2)	10(1)	neg5(3)	0.1190	2120.447	120.209	5
4N/O	2.12(9)	30(40)					
3S	2.23(2)	6(1)	6(7)	0.2139	3810.473	216.018	5
3N/O	2.14(0.19)	33(90)					
4S	2.21(3)	9(2)	2(9)	0.2620	4666.760	264.561	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	1.84(3)	4(2)					5
1Br	2.27(2)	3(1)	neg18(6)	0.2613	4654.853	263.886	
1N/O	1.83(2)	0(2)					5
2Br	2.26(2)	6(1)	neg20(5)	0.2309	4112.025	233.113	
2N/O	1.83(2)	3(2)	neg20(5)	0.2101	3742.863	212.185	5

2Br	2.27(2)	6(1)					
3N/O	1.85(3)	6(2)					
1Br	2.27(2)	3(1)	neg17(6)	0.2489	4433.732	251.350	5
1N/O	1.82(2)	0(1)					
3Br	2.26(2)	9(1)	neg21(5)	0.2106	3752.032	212.704	5
1N/O	1.82(2)	0(1)					
4Br	2.27(2)	10(1)	neg21(5)	0.2054	3658.139	207.382	5
4N/O	1.85(3)	9(3)					
1Br	2.28(2)	3(1)	neg16(6)	0.2452	4368.002	247.624	5
2N/O	1.82(2)	3(1)					
3Br	2.27(2)	8(1)	neg20(4)	0.1998	3558.643	201.741	5
3N/O	1.83(2)	6(2)					
2Br	2.27(2)	6(1)	neg19(5)	0.2100	3740.778	212.066	5
5N/O	1.86(4)	11(3)					
1Br	2.28(2)	3(1)	neg15(6)	0.2455	4373.067	247.911	5
1N/O	1.82(2)	0(1)					
5Br	2.27(2)	12(1)	neg22(5)	0.2065	3678.012	208.508	5
4N/O	1.83(3)	8(2)					
2Br	2.27(2)	6(1)	neg19(5)	0.2162	3851.819	218.361	5
2N/O	1.82(2)	3(1)					
4Br	2.27(2)	10(1)	neg21(4)	0.2024	3605.570	204.401	5
3N/O	1.82(2)	5(2)					
3Br	2.27(2)	8(1)	neg20(4)	0.2077	3698.893	209.692	5
6N/O	1.86(4)	13(4)					
1Br	2.28(2)	3(1)	neg14(6)	0.2477	4411.350	250.082	5
1N/O	1.82(2)	0(1)					
6Br	2.27(2)	13(1)	neg22(5)	0.2106	3751.550	212.672	5
5N/O	1.83(3)	11(3)					
2Br	2.27(2)	6(1)	neg18(5)	0.2234	3979.285	225.588	5
2N/O	1.82(2)	3(1)					
5Br	2.27(2)	12(1)	neg21(4)	0.2100	3740.114	212.029	5
4N/O	1.82(3)	8(2)					
3Br	2.27(2)	8(1)	neg20(5)	0.2192	3905.029	221.378	5

3N/O	1.82(2)	5(2)					
4Br	2.27(2)	10(1)	neg21(5)	0.2158	3843.265	217.877	5

Ni-N(2.0) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(2)	4(1)					
1Imd	1.89(2)	1(1)	10(2)	0.3671	6539.389	370.721	5
4N/O	2.00(5)	13(7)					
1Imd	2.11(2)	3(2)					
1Imd	1.97(5)	1(6)	8(2)	0.2614	4655.404	297.667	7
3N/O	1.95(7)	19(13)					
1Imd	2.13(2)	9(1)					
1Imd	1.90(2)	6(2)					
1Imd	2.01(2)	9(2)	6(2)	0.2133	3798.792	278.511	9
2N/O	2.09(2)	0(2)					
1Imd	2.11(3)	6(2)					
1Imd	1.63(0.13)	20(21)					
1Imd	1.98(3)	8(2)					
1Imd	1.86(2)	5(2)	9(2)	0.1728	3078.487	264.483	11
1N/O	2.10(2)	3(2)					
1Imd	1.55(0.17)	15(18)					
1Imd	2.00(3)	10(4)					
1Imd	1.82(0.13)	6(34)					
1Imd	2.11(2)	9(3)					
1Imd	1.88(4)	7(5)	8(3)	0.1535	2733.587	283.577	13
4N/O	2.02(3)	9(3)					
1Imd	2.11(1)	2(1)	11(2)	0.2835	5050.331	286.306	5
3N/O	2.07(2)	3(2)					
1Imd	1.92(2)	1(2)					
1Imd	2.09(4)	1(3)	11(2)	0.2451	4365.397	279.124	7
2N/O	2.09(2)	0(2)					
1Imd	1.87(2)	6(2)					
1Imd	2.10(2)	6(2)					
1Imd	1.98(2)	8(2)	8(2)	0.1967	3503.768	256.881	9
1N/O	2.10(2)	3(2)					
1Imd	2.11(2)	8(2)					
1Imd	1.88(2)	6(2)					
1Imd	1.99(2)	9(2)					
1Imd	1.60(0.16)	26(31)	9(2)	0.1578	2810.593	241.467	11
0N/O			3(2)	0.2152	3833.064	329.311	11

1Imd	2.13(2)	14(2)					
1Imd	2.03(2)	17(2)					
1Imd	1.93(3)	16(2)					
1Imd	1.75(7)	1(9)					
1Imd	1.83(3)	12(3)					
3N/O	2.03(3)	6(3)					
1Imd	2.12(1)	2(1)	13(2)	0.2896	5158.254	292.424	5
2N/O	2.09(2)	0(2)					
1Imd	1.93(2)	2(1)					
1Imd	2.09(3)	1(2)	11(2)	0.2169	3863.691	247.045	7
1N/O	2.10(2)	3(1)					
1Imd	1.99(2)	9(2)					
1Imd	2.11(2)	8(2)					
1Imd	1.88(2)	6(2)	8(2)	0.1678	2989.220	219.157	9
0N/O							
1Imd	1.84(2)	9(3)					
1Imd	2.15(2)	12(2)					
1Imd	1.94(2)	13(3)					
1Imd	2.04(2)	14(3)	6(2)	0.2350	4186.178	306.912	9
2N/O	2.05(3)	4(4)					
1Imd	2.13(2)	2(1)	15(3)	0.3176	5657.016	320.699	5
1N/O	2.09(2)	3(2)					
1Imd	2.11(3)	2(2)					
1Imd	1.96(2)	2(2)	12(2)	0.2277	4056.256	259.357	7
0N/O							
1Imd	2.13(1)	9(1)					
1Imd	2.01(2)	10(1)					
1Imd	1.90(2)	7(2)	8(2)	0.2527	4501.264	287.811	7

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(4)	4(4)					
1S	2.21(1)	0(0)					
1Imd	1.94(3)	2(3)	0(2)	0.0826	1470.857	94.047	7
0N/O							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.88(4)	4(4)					
1S	2.21(1)	0(0)					
1Imd	1.94(3)	2(3)	0(2)	0.0802	1427.674	91.286	7
0N/O							
1S	2.22(1)	0(1)					
1Imd	2.00(3)	1(2)					
1Imd	1.88(2)	1(2)	1(2)	0.0726	1293.161	82.685	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(5)	5(5)					
1S	2.21(1)	0(0)					
1Imd	1.94(3)	3(3)	0(2)	0.0782	1392.077	89.009	7
0N/O							
1S	2.22(1)	0(1)					
1Imd	1.88(2)	1(1)					
1Imd	2.01(2)	1(2)	2(2)	0.0625	1112.636	71.142	9

Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.20(1)	3(0)					
1Imd	1.89(1)	0(1)	neg2(1)	0.0678	1208.029	68.484	5

Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.20(1)	3(0)					
1Imd	1.88(1)	0(1)	neg3(1)	0.0649	1155.574	65.510	5

Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.20(1)	3(0)					
1Imd	4	0(1)	neg3(1)	0.0617	1099.910	62.354	5

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.91(4)	9(5)					
1S	2.21(1)	0(0)					
1Imd	1.94(3)	3(3)	0(2)	0.0715	1273.781	81.446	7
1N/O	1.84(3)	2(3)					
1S	2.22(1)	0(1)	1(2)	0.0537	955.702	70.068	9

1Imd	1.92(3)	1(2)					
1Imd	2.04(3)	1(3)					

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.91(4)	9(5)					
1S	2.21(1)	0(0)					
1Imd	1.94(3)	3(3)	0(2)	0.0696	1239.562	79.258	7
1N/O	1.84(3)	2(3)					
1S	2.22(1)	0(1)					
1Imd	1.92(3)	1(2)					
1Imd	2.04(3)	1(3)	1(2)	0.0516	918.659	67.352	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	1.92(5)	10(5)					
1S	2.21(1)	0(0)					
1Imd	1.93(3)	3(3)	0(2)	0.0676	1203.414	76.946	7
1N/O	1.89(6)	8(8)					
1S	2.22(1)	0(1)					
1Imd	2.03(3)	0(2)					
1Imd	1.90(2)	0(2)	2(2)	0.0467	831.049	60.929	9

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.05(3)	4(4)					
1S	2.77(4)	5(5)					
1Imd	2.13(2)	2(1)	15(3)	0.2841	5060.004	323.537	7
1N/O	2.09(2)	3(2)					
1S	2.81(0.12)	15(19)					
1Imd	1.95(2)	2(2)					
1Imd	2.11(3)	2(2)	13(2)	0.2143	3817.369	279.873	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(3)	4(4)					
1S	2.77(4)	5(5)					
1Imd	2.13(2)	2(1)	15(3)	0.2874	5119.849	327.363	7
1N/O	2.09(2)	3(2)					
1S	2.88(0.21)	23(39)	13(2)	0.2159	3845.560	281.940	9

1Imd	2.11(3)	2(2)					
1Imd	1.96(2)	2(2)					

Ni-N(2.0) Ni-S(2.2) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	3(2)					
2S	2.20(1)	3(0)					
1Imd	1.91(2)	1(1)	neg2(1)	0.0497	884.932	56.583	7
0N/O							
2S	2.21(1)	3(1)					
1Imd	1.99(4)	4(6)					
1Imd	1.87(2)	0(2)	neg1(2)	0.0554	987.652	63.151	9

Ni-N(2.0) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(2)	3(3)					
2S	2.20(1)	3(0)					
1Imd	1.91(2)	1(1)	neg3(1)	0.0493	878.007	56.140	7
0N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.84(3)	3(3)					
2S	2.20(1)	3(0)					
1Imd 0°	1.90(2)	1(1)	neg3(1)	0.05	891.197	56.983	7
1N/O	1.83(3)	3(3)					
2S	2.20(1)	3(0)					
1Imd 5°	1.91(2)	1(2)	neg3(2)	0.0546	973.291	62.232	7
1N/O	1.87(1)	1(1)					
2S	2.22(1)	4(1)					
1Imd 10°	2.02(2)	1(2)	1(2)	0.0674	1200.806	76.780	7
0N/O							
2S	2.21(1)	3(1)					
1Imd 0°	1.87(1)	0(2)					
1Imd 0°	1.98(4)	3(5)	neg1(2)	0.0494	879.945	56.264	7
0N/O							
2S	2.21(1)	4(1)	neg1(2)	0.0503	895.218	57.240	7

1Imd 0°	1.87(1)	0(1)					
1Imd 5°	2.00(4)	2(4)					
0N/O							
2S	2.20(1)	3(1)					
1Imd 0°	1.88(1)	0(1)					
1Imd 10°	1.88(0.12)	15(13)	neg3(2)	0.0562	1001.930	64.063	7
0N/O							
2S	2.20(1)	3(1)					
1Imd 5°	1.88(1)	0(1)					
1Imd 10°	1.89(0.15)	16(16)	neg3(2)	0.0623	1109.266	70.927	7

Ni-N(2.0) Ni-S(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.13(2)	3(1)					
2S	2.95(0.23)	35(49)					
1Imd	2.06(7)	3(6)	18(5)	0.335	5967.281	381.548	7
0N/O							
2S	2.99(0.25)	33(50)					
1Imd	1.99(3)	2(3)					
1Imd	2.11(2)	4(2)	13(3)	0.3786	6744.463	431.241	9

Ni-N(2.0) Ni-S(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.13(2)	3(1)					
2S	2.98(0.25)	37(54)					
1Imd	2.05(6)	3(6)	18(4)	0.3331	5933.863	379.412	7
0N/O							
2S	3.03(0.19)	28(38)					
1Imd	1.99(4)	2(3)					
1Imd	2.12(2)	4(2)	13(3)	0.3769	6714.220	429.308	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(2)	2(2)					
1S	2.15(3)	1(3)					
1S	2.24(2)	0(2)					
1Imd 0°	1.91(2)	1(2)	neg3(2)	0.0477	850.436	62.350	9
1N/O	1.83(2)	1(2)					
1S	2.14(3)	1(3)					
1S	2.24(2)	0(2)					
1Imd 5°	1.92(3)	1(2)	neg3(2)	0.0514	914.962	67.081	9

1N/O	1.86(2)	1(1)					
1S	2.14(3)	5(7)					
1S	2.24(2)	0(1)					
1Imd 10°	2.02(2)	1(1)	0(2)	0.0491	874.358	64.104	9
0N/O							
1S	2.22(2)	1(1)					
1S	2.17(5)	8(7)					
1Imd	2.00(3)	1(3)					
1Imd	1.87(2)	0(2)	0(2)	0.0432	769.123	56.389	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(2)	2(2)					
1S	2.24(2)	0(2)					
1S	2.15(2)	1(3)					
1Imd	1.91(2)	1(2)	neg4(2)	0.0472	840.750	61.640	9
0N/O							
1S	2.22(2)	0(1)					
1S	2.16(4)	7(7)					
1Imd	1.99(3)	1(4)					
1Imd	1.86(2)	0(2)	neg2(2)	0.0464	825.868	60.549	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(5)	4(5)					
1S	2.21(1)	0(0)					
1S	2.70(6)	12(8)					
1Imd	1.94(4)	3(4)	0(2)	0.0767	1366.315	100.172	9
0N/O							
1S	2.22(1)	0(1)					
1S	2.76(0.10)	18(16)					
1Imd	2.00(3)	1(3)					
1Imd	1.88(2)	1(2)	1(2)	0.0725	1291.500	94.687	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(5)	4(5)					
1S	2.21(1)	0(0)					
1S	2.70(6)	13(8)					
1Imd	1.94(4)	3(4)	0(2)	0.0771	1373.029	100.665	9
0N/O							
1S			No Fit	No Fit	No Fit	No Fit	9

1S							
1Imd							
1Imd							

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.83(2)	2(2)					
1S	2.15(4)	2(4)					
1S	2.23(3)	0(2)					
1Imd	1.90(2)	1(2)	neg4(2)	0.0472	840.871	61.649	9
0N/O							
1S	2.22(2)	0(1)					
1S	2.16(4)	8(7)					
1Imd	1.86(2)	0(2)					
1Imd	1.99(3)	1(4)	neg2(2)	0.0453	806.692	59.143	9

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(5)	5(5)					
1S	2.21(1)	0(0)					
1S	2.69(6)	13(8)					
1Imd	1.93(4)	3(3)	neg1(2)	0.0752	1339.563	98.211	9
0N/O							
1S	2.22(2)	1(1)					
1S	2.16(4)	8(7)					
1Imd 0°	1.99(3)	1(4)					
1Imd 0°	1.86(2)	0(2)	neg2(2)	0.0451	802.685	58.849	9
0N/O							
1S	2.21(1)	0(1)					
1S	2.73(7)	14(10)					
1Imd 0°	1.98(3)	1(3)					
1Imd 5°	1.87(2)	1(2)	0(2)	0.072	1281.695	93.968	9
0N/O							
1S	2.22(1)	0(1)					
1S	2.79(5)	8(6)					
1Imd 0°	1.89(2)	1(1)					
1Imd 10°	2.02(3)	1(2)	2(2)	0.0755	1344.070	98.541	9
0N/O							
1S	2.22(1)	0(1)					
1S	2.12(3)	7(8)					
1Imd 5°	1.88(2)	1(1)					
1Imd 10°	2.03(2)	0(2)	neg2(2)	0.0541	963.888	70.668	9

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(5)	5(5)					
1S	2.21(1)	0(0)					
1S	2.70(7)	13(9)					
1Imd	1.93(4)	3(4)	ne1(2)	0.0756	1345.812	98.669	9
0N/O							
1S							
1S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(5)	5(5)					
1S	2.68(7)	13(9)					
1S	2.21(1)	0(0)					
1Imd	1.93(4)	3(3)	neg2(2)	0.0722	1286.615	94.329	9
0N/O							
1S	2.97(0.37)	29(70)					
1S	1.73(4)	13(6)					
1Imd	2.02(4)	0(5)					
1Imd	2.13(2)	3(2)	14(3)	0.2689	4789.948	351.178	9

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.89(5)	5(5)					
1S	2.21(1)	0(0)					
1S	2.69(7)	13(9)					
1Imd	1.93(4)	3(3)	neg1(2)	0.0743	1323.625	97.042	9
0N/O							
1S	2.22(1)	0(1)					
1S	2.78(0.12)	22(21)					
1Imd	1.99(3)	1(3)					
1Imd	1.87(2)	1(2)	0(2)	0.068	1212.114	88.867	9

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6) Ni-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.03(4)	0(4)					
1S	2.82(7)	8(10)	16(4)	0.2516	4481.437	328.560	9

1S	3.10(3)	1(2)					
1Imd	2.13(2)	4(2)					
0N/O							
1S	2.62(5)	2(4)					
1S	2.79(4)	0(3)					
1Imd	1.96(3)	1(3)					
1Imd	2.10(2)	4(2)	10(0)	0.4006	7135.828	523.168	9

APPENDIX K

ADDITIONAL FIT TABLES FOR PHD2

Table K.1. Additional Fits for Ni(II) WT-PHD2 in Buffer with 50 mM PBS, 150 mM NaBr at pH 7.2.

Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	1(2)	4(9)	0.3384	4941.824	727.073	3
3N/O	2.08(2)	0(2)	4(6)	0.2256	3294.244	484.670	3
4N/O	2.08(2)	2(1)	4(4)	0.1563	2282.434	335.806	3
5N/O	2.08(2)	3(1)	4(3)	0.1174	1714.306	252.220	3
6N/O	2.08(2)	4(1)	3(2)	0.1007	1470.964	216.378	3
7N/O	2.09(2)	5(1)	3(2)	0.1005	1467.907	215.968	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.17(4)	3(2)	neg19(10)	0.2900	4235.234	623.115	3
3S	2.17(3)	5(2)	neg18(7)	0.2103	3071.021	451.828	3
4S	2.18(3)	6(1)	neg18(6)	0.1693	2472.755	363.808	3
5S	2.18(3)	8(1)	neg17(5)	0.1509	2204.454	324.333	3
6S	2.19(3)	9(1)	neg17(5)	0.1464	2138.464	314.625	3
7S	2.19(3)	11(2)	neg17(5)	0.1505	2198.457	323.451	3

Ni-N(2.0) Ni-N(2.2)

N	Radius Å	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.14(3)	6(2)					
1N/O	2.01(2)	8(2)	5(5)	0.1435	2096.165	436.985	5
2N/O	2.03(2)	5(1)					
2N/O	2.17(2)	4(2)	5(3)	0.0794	1159.402	241.699	5
3N/O	2.06(2)	3(1)					
1N/O	2.20(2)	7(2)	5(3)	0.0809	1181.668	246.341	5
4N/O	2.07(2)	1(1)					
1N/O	2.21(2)	5(2)	5(2)	0.0657	960.099	200.151	5
3N/O	2.05(2)	2(1)					
2N/O	2.18(2)	3(2)	5(2)	0.0665	971.187	202.462	5
5N/O	2.07(2)	1(1)					
1N/O	2.22(3)	4(2)	5(2)	0.0690	1008.180	210.174	5
4N/O	2.06(2)	0(2)	5(2)	0.0719	1050.616	219.021	5

2N/O	2.19(3)	2(3)					
3N/O	2.04(2)	1(2)					
3N/O	2.17(3)	0(3)	4(2)	0.0741	1082.644	225.698	5
6N/O	2.08(2)	2(1)					
1N/O	2.23(4)	3(3)	4(3)	0.0844	1232.955	257.033	5
5N/O	2.06(2)	1(2)					
2N/O	2.20(4)	0(4)	4(3)	0.0886	1294.610	269.886	5
4N/O	2.05(2)	1(2)					
3N/O	2.18(4)	2(5)	4(3)	0.0912	1331.887	277.657	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.16(3)	1(2)					
1S	2.29(4)	3(2)	neg14(7)	0.1338	1953.453	407.235	5
2S	2.14(3)	0(2)					
2S	2.28(4)	1(2)	neg14(6)	0.1148	1676.731	349.547	5
3S	2.17(3)	2(1)					
1S	2.31(4)	2(2)	neg14(6)	0.1152	1681.879	350.620	5
4S	2.18(3)	4(1)					
1S	2.33(4)	0(3)	neg14(5)	0.1132	1653.634	344.732	5
3S	2.16(3)	2(2)					
2S	2.30(4)	2(3)	neg14(5)	0.1127	1645.882	343.116	5
5S	2.18(3)	6(2)					
1S	2.34(5)	1(4)	neg14(5)	0.1196	1746.787	364.151	5
4S	2.17(3)	4(2)					
2S	2.32(5)	4(4)	neg14(6)	0.1183	1727.855	360.204	5
3S	2.16(3)	3(2)					
3S	2.29(5)	6(4)	neg13(6)	0.1172	1712.269	356.955	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.18(3)	6(2)					
2S	2.34(7)	6(6)	neg13(6)	0.1260	1839.792	383.540	5
4S	2.17(3)	5(3)					
3S	2.32(7)	8(7)	neg13(6)	0.1238	1807.724	376.854	5

Ni-N(2.0) Ni-S(2.2)							
N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.03(3)	3(2)					5
1S	2.29(4)	0(2)	neg2(6)	0.1324	1932.944	402.959	
1N/O	2.00(3)	4(2)					5
2S	2.25(4)	3(2)	neg7(7)	0.1446	2112.194	440.327	
2N/O	2.02(3)	1(2)					
2S	2.27(4)	4(3)	neg4(6)	0.1167	1704.418	355.318	5
3N/O	2.04(2)	1(1)					
1S	2.30(4)	1(3)	neg1(5)	0.1013	1479.234	308.375	5
1N/O	2.00(3)	3(2)					
3S	2.24(4)	6(2)	neg8(6)	0.1233	1800.466	375.341	5
1N/O	1.87(0.60)	17(84)					
4S	2.18(4)	6(2)	neg18(11)	0.1640	2395.622	499.413	5
4N/O	2.05(2)	1(1)					
1S	2.31(4)	2(3)	0(4)	0.0909	1327.924	276.831	5
2N/O	2.02(3)	1(2)					
3S	2.26(4)	8(3)	neg6(6)	0.1127	1645.862	343.111	5
3N/O	2.04(3)	1(2)					
2S	2.29(4)	6(4)	neg3(5)	0.1052	1536.285	320.268	5
5N/O	2.06(2)	3(2)					
1S	2.31(5)	5(5)	0(4)	0.0932	1361.864	283.906	5
1N/O	3.25(3)	9(3)					
5S	2.19(3)	8(2)	neg15(5)	0.1225	1789.571	373.070	5
4N/O	2.05(3)	2(2)					
2S	2.29(6)	9(5)	neg2(5)	0.1027	1499.944	312.692	5
2N/O	2.47(6)	1(4)					
4S	2.16(3)	6(2)	neg20(6)	0.1305	1905.525	397.243	5
3N/O	2.04(3)	1(2)					
3S	2.27(5)	10(4)	neg4(6)	0.1088	1589.567	331.376	5
6N/O	2.09(1)	4(1)					
1S	2.65(3)	2(3)	5(2)	0.0581	848.364	176.858	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5

5N/O	2.07(3)	4(2)					
2S	2.30(9)	14(10)	0(5)	0.1035	1511.592	315.120	5
2N/O	2.65(0.27)	13(42)					
5S	2.19(3)	8(2)	neg16(6)	0.1403	2049.382	427.233	5
4N/O	2.05(3)	3(2)					
3S	2.28(7)	14(7)	neg2(5)	0.1076	1571.210	327.549	5
3N/O	3.10(8)	1(7)					
4S	2.17(2)	6(1)	neg19(5)	0.1143	1668.877	347.909	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.06(3)	2(2)					5
1Br	2.43(5)	5(3)	3(9)	0.2169	3168.028	660.436	
1N/O	1.97(7)	4(3)					5
2Br	2.31(0.10)	7(3)	neg24(24)	0.3879	5664.755	1180.926	
2N/O	2.06(4)	2(2)					
2Br	2.43(6)	9(4)	2(10)	0.2360	3446.721	718.535	5
3N/O	2.07(2)	0(1)					
1Br	2.44(4)	5(3)	3(6)	0.1392	2032.947	423.807	5
1N/O	2.18(7)	5(3)					
3Br	2.24(6)	6(3)	neg45(17)	0.2844	4153.355	865.846	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.07(2)	1(1)					
1Br	2.44(4)	6(3)	3(4)	0.0976	1425.607	297.195	5
2N/O	2.06(4)	1(2)					
3Br	2.44(7)	13(5)	2(10)	0.2536	3704.211	772.213	5
3N/O	2.07(3)	0(2)					
2Br	2.44(5)	10(4)	2(6)	0.1616	2359.981	491.983	5
5N/O	2.07(2)	3(1)					
1Br	2.44(3)	7(3)	3(3)	0.0794	1159.708	241.763	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.07(2)	2(2)					
2Br	2.44(5)	12(4)	3(4)	0.1191	1739.000	362.528	5

2N/O	1.37(0.10)	6(9)					
4Br	2.20(6)	9(2)	neg49(17)	0.2983	4356.800	908.258	5
3N/O	2.07(3)	0(2)					
3Br	2.44(6)	14(5)	3(7)	0.1787	2609.145	543.926	5
6N/O	2.08(2)	4(1)					
1Br	2.43(4)	9(4)	3(3)	0.0764	1115.862	232.623	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.08(2)	3(1)					
2Br	2.43(5)	14(5)	3(4)	0.0964	1407.941	293.512	5
2N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.08(2)	2(2)					
3Br	2.44(6)	16(6)	3(5)	0.1328	1939.552	404.336	5
3N/O	2.07(3)	1(2)					
4Br	2.44(7)	17(6)	3(7)	0.1914	2795.760	582.830	5

Table K.2. Additional Fits for Ni(II) WT-PHD2 in Buffer with 50 mM Hepes, 150 mM NaBr at pH 7.2.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	1(1)	4(6)	0.3516	4559.614	271.440	3
3N/O	2.08(2)	0(1)	4(4)	0.2427	3679.626	219.053	3
4N/O	2.08(1)	2(1)	4(3)	0.1763	2672.548	159.101	3
5N/O	2.08(1)	3(1)	4(2)	0.1395	2114.599	125.885	3
6N/O	2.08(1)	4(1)	3(2)	0.1243	1884.205	112.169	3
7N/O	2.09(1)	5(1)	3(2)	0.1250	1896.076	112.876	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.16(2)	3(1)	neg19(7)	0.3037	4605.028	274.144	3
3S	2.17(2)	5(1)	neg18(5)	0.2275	3448.871	205.316	3
4S	2.18(2)	6(1)	neg18(4)	0.1887	2861.566	170.353	3
5S	2.18(2)	8(1)	neg18(4)	0.1717	2604.055	155.023	3
6S	2.18(2)	9(1)	neg17(3)	0.1680	2547.761	151.672	3
7S	2.19(2)	11(1)	neg17(3)	0.1725	2616.169	155.744	3

Ni-N(2.0) Ni-N(2.2)

N	Radius Å	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.13(2)	5(2)					
1N/O	2.01(2)	8(1)	5(3)	0.1828	2771.602	187.298	5
2N/O	2.04(1)	4(1)					
2N/O	2.16(2)	4(1)	5(2)	0.1168	1771.424	119.708	5
3N/O	2.13(2)	3(1)					
1N/O	2.01(2)	6(1)	5(2)	0.1318	1999.187	135.100	5
4N/O	2.07(1)	1(1)					
1N/O	2.21(2)	4(2)	5(2)	0.1018	1543.713	104.320	5
3N/O	2.05(1)	2(1)					
2N/O	2.18(2)	3(2)	5(2)	0.1009	1530.574	103.432	5
5N/O	2.07(1)	1(1)					
1N/O	2.22(2)	3(2)	5(2)	0.1019	1545.537	104.443	5
4N/O	2.06(1)	0(1)					
2N/O	2.19(2)	1(2)	4(2)	0.1033	1565.734	105.808	5
3N/O	2.04(2)	1(1)					
3N/O	2.17(2)	1(2)	4(2)	0.1041	1578.448	106.667	5
6N/O	2.08(1)	3(1)					
1N/O	2.23(3)	2(3)	4(2)	0.1141	1730.344	116.932	5
5N/O	2.07(1)	2(1)					
2N/O	2.20(3)	1(3)	4(2)	0.1168	1771.001	119.680	5
4N/O	2.05(2)	1(2)					
3N/O	2.17(3)	3(4)	4(2)	0.1180	1789.966	120.961	5

Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.16(2)	0(1)					
1S	2.30(3)	2(1)	neg14(4)	0.1636	2480.188	167.605	5
2S	2.15(2)	0(1)					
2S	2.28(3)	1(2)	neg13(4)	0.1408	2135.706	144.325	5
3S	2.17(2)	2(1)					
1S	2.32(3)	1(2)	neg14(4)	0.1408	2135.493	144.311	5
4S	2.18(2)	4(1)					
1S	2.33(3)	0(2)	neg14(3)	0.1359	2061.196	139.290	5

3S	2.16(2)	2(1)					
2S	2.30(3)	2(2)	neg13(3)	0.1356	2056.361	138.963	5
5S	2.19(2)	6(1)					
1S	2.35(3)	1(2)	neg14(3)	0.1404	2128.758	143.856	5
4S	2.17(2)	4(1)					
2S	2.32(3)	4(2)	neg13(3)	0.1393	2112.031	142.726	5
3S	2.16(2)	3(1)					
3S	2.30(3)	6(3)	neg13(3)	0.1384	2098.753	141.828	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.18(2)	6(1)					
2S	2.35(4)	6(3)	neg13(4)	0.1463	2217.886	149.879	5
4S	2.17(2)	5(2)					
3S	2.32(4)	8(4)	neg13(4)	0.1442	2186.747	147.775	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.04(2)	2(1)					5
1S	2.29(3)	0(2)	neg1(4)	0.1673	2536.238	171.392	
1N/O	2.00(2)	4(1)					5
2S	2.25(3)	3(2)	neg7(5)	0.1790	2714.883	183.465	
2N/O	2.03(2)	1(1)					
2S	2.27(3)	5(2)	neg4(4)	0.1466	2223.060	150.229	5
3N/O	2.05(2)	0(1)					
1S	2.30(3)	1(2)	0(3)	0.1318	1998.092	135.026	5
1N/O	2.01(2)	3(1)					
3S	2.24(3)	6(2)	neg9(4)	0.1537	2330.106	157.462	5
1N/O	1.85(0.26)	16(43)					
4S	2.18(2)	6(1)	neg19(6)	0.1835	2781.797	187.987	5
4N/O	2.06(1)	1(1)					
1S	2.31(3)	3(2)	0(3)	0.1183	1793.925	121.229	5
2N/O	2.03(2)	0(1)					
3S	2.26(3)	8(2)	neg6(4)	0.1396	2117.011	143.062	5
3N/O	2.04(2)	1(1)					
2S	2.29(3)	6(2)	neg2(3)	0.1316	1995.020	134.818	5

5N/O	2.06(2)	3(1)					
1S	2.32(4)	5(4)	1(2)	0.1185	1797.137	121.446	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.05(2)	2(1)					
2S	2.30(4)	9(4)	neg1(3)	0.1270	1925.690	130.133	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
3N/O	2.04(2)	1(1)					
3S	2.28(4)	10(3)	neg4(4)	0.1334	2022.794	136.695	5
6N/O	2.09(1)	4(1)					
1S	2.66(2)	2(2)	5(1)	0.0768	1164.914	78.722	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.07(2)	4(1)					
2S	2.30(6)	15(7)	0(3)	0.1269	1924.262	130.037	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.06(2)	3(1)					
3S	2.29(5)	14(5)	neg2(3)	0.1309	1985.500	134.175	5
3N/O	1.85(0.18)	23(30)					
4S	2.17(2)	6(1)	neg19(6)	0.1789	2712.837	183.326	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.07(2)	2(1)					5
1Br	2.43(3)	5(2)	3(5)	0.2356	3572.794	241.440	
1N/O	2.05(3)	5(1)					5
2Br	2.42(5)	9(3)	1(10)	0.3792	5749.661	388.547	
2N/O	2.06(2)	2(1)					
2Br	2.43(3)	9(2)	2(5)	0.2501	3792.416	256.282	5
3N/O	2.07(1)	0(1)					
1Br	2.44(2)	6(2)	3(3)	0.1581	2396.653	161.959	5
1N/O							
3Br			No Fit	No Fit	No Fit	No Fit	5

1N/O 4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 1Br	2.07(1) 2.44(2)	1(1) 6(2)	3(2)	0.1172	1776.663	120.062	5
2N/O 3Br	2.06(2) 2.44(4)	2(1) 12(3)	2(6)	0.2668	4045.355	273.374	5
3N/O 2Br	2.07(2) 2.44(3)	0(1) 10(2)	3(4)	0.1776	2693.248	182.003	5
5N/O 1Br	2.08(1) 2.44(2)	3(1) 7(2)	3(2)	0.1001	1517.128	102.524	5
1N/O 5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O 2Br	2.07(1) 2.44(3)	2(1) 12(3)	3(3)	0.1374	2083.327	140.786	5
2N/O 4Br	2.06(2) 2.44(4)	1(1) 15(3)	2(6)	0.2821	4277.221	289.043	5
3N/O 3Br	2.07(2) 2.44(3)	0(1) 14(3)	3(4)	0.1949	2955.691	199.738	5
6N/O 1Br	2.08(1) 2.44(3)	4(1) 9(3)	3(2)	0.0984	1492.438	100.855	5
1N/O 6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O 2Br	2.08(1) 2.43(3)	3(1) 13(3)	3(2)	0.1170	1773.965	119.880	5
2N/O 5Br	2.07(2) 2.44(5)	1(1) 17(4)	2(6)	0.2954	4479.801	302.733	5
4N/O 3Br	2.08(2) 2.44(3)	2(1) 16(4)	3(3)	0.1520	2305.286	155.785	5
3N/O 4Br	2.07(2) 2.44(4)	1(1) 17(4)	3(4)	0.2088	3165.730	213.932	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)	5(1)	0.0371	563.015	43.993	7

1S	2.51(1)	9(1)					
1Br	2.46(1)	5(1)					
3N/O	2.07(1)	1(1)					
2S	2.44(5)	10(6)					
1Br	2.42(2)	4(2)	4(2)	0.0757	1147.112	89.633	7
2N/O	2.05(1)	2(1)					
3S	2.37(4)	11(5)					
1Br	2.38(3)	5(2)	1(3)	0.0982	1488.323	116.295	7
1N/O							
4S							
1Br			No Fit	No Fit	No Fit	No Fit	7
3N/O	2.07(1)	0(1)					
1S	2.41(6)	0(4)					
2Br	2.40(4)	7(4)	3(2)	0.0902	1367.461	106.851	7
2N/O							
1S							
3Br			No Fit	No Fit	No Fit	No Fit	7
1N/O	2.02(3)	4(2)					
1S	2.26(4)	0(3)					
4Br	1.95(0.10)	24(9)	7(8)	0.1982	3004.820	234.791	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(2)	8(1)					
1Br	2.46(1)	4(1)	5(1)	0.0353	535.054	41.808	7
4N/O	2.08(1)	1(1)					
2S	2.49(4)	10(5)					
1Br	2.44(2)	4(2)	5(1)	0.0523	792.945	61.959	7
3N/O	2.07(1)	1(1)					
3S	2.45(4)	15(5)					
1Br	2.43(2)	4(1)	4(2)	0.0642	973.503	76.068	7
2N/O	2.05(1)	2(1)					
4S	2.39(4)	15(5)					
1Br	2.40(2)	5(2)	1(3)	0.0870	1318.578	103.031	7
4N/O	2.08(1)	2(1)					
1S	2.42(4)	1(3)					
2Br	2.40(3)	6(3)	3(2)	0.0620	939.497	73.411	7

3N/O	2.08(2)	0(1)					
1S	2.38(4)	0(2)					
3Br	2.37(4)	11(4)	3(2)	0.0931	1411.861	110.320	7
2N/O	2.15(3)	2(3)					
1S	1.89(2)	3(2)					
4Br	2.45(3)	20(5)	13(3)	0.1309	1984.800	155.089	7

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.09(1)	4(1)					
1S	2.66(2)	2(2)	5(1)	0.0768	1164.914	78.722	5

Ni-N(2.0) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.07(2)	4(1)					
1S	2.31(8)	13(12)	1(3)	0.1250	1895.749	128.110	5

Ni-N(2.0) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.09(1)	4(1)					
1S	2.66(2)	2(2)	5(1)	0.0706	1069.876	72.299	5

Ni-N(2.0) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.09(1)	4(1)					
1S	2.66(2)	2(2)	5(1)	0.0682	1033.468	69.839	5

Ni-N(2.0) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.09(1)	4(1)					
1S	2.66(2)	2(2)	5(1)	0.0667	1011.154	68.331	5

Ni-N(2.0) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.08(1)	4(1)					
1Br	2.44(3)	9(3)	3(2)	0.0984	1276.285	86.248	5

Ni-N(2.0) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.08(1)	4(1)					
1Br	2.44(3)	9(3)	3(2)	0.0965	1463.785	98.919	5

Ni-N(2.0) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.08(1)	4(1)					
1Br	2.44(2)	9(3)	3(2)	0.0950	1439.787	97.297	5

Ni-N(2.0) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.08(1)	4(1)					
1Br	3.27(0.21)	19(28)	3(2)	0.1203	1823.508	123.228	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.05(2)	2(1)					
2S	2.30(4)	9(4)	neg1(3)	0.1270	1925.690	130.133	5

Ni-N(2.0) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.05(2)	2(1)					
2S	2.30(4)	9(4)	neg2(3)	0.1299	1970.062	133.132	5

Ni-N(2.0) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.05(2)	2(1)					
2S	2.30(4)	10(4)	neg2(3)	0.1324	2007.155	135.638	5

Ni-N(2.0) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	2(1)					
2S	2.47(0.15)	29(21)	3(3)	0.1494	2266.094	153.137	5

Ni-N(2.0) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(1)	2(1)					
2S	2.67(3)	8(3)	6(2)	0.1453	2202.613	148.847	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(2)	4(1)					
2S	2.30(6)	15(7)	0(3)	0.1269	1924.262	130.037	5

Ni-N(2.0) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(2)	3(1)					
2S	2.31(6)	15(7)	0(3)	0.1288	1953.642	132.022	5

Ni-N(2.0) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(1)	3(1)					
2S	2.66(3)	8(3)	6(2)	0.1108	1679.707	113.510	5

Ni-N(2.0) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(1)	3(1)					
2S	2.66(2)	8(3)	6(2)	0.1077	1633.721	110.403	5

Ni-N(2.0) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(1)	3(1)					
2S	2.66(2)	9(3)	6(2)	0.1059	1605.416	108.490	5

Ni-N(2.0) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	3(1)					
2Br	2.43(3)	13(3)	3(2)	0.1170	1773.965	119.880	5

Ni-N(2.0) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	3(1)					
2Br	2.44(3)	13(3)	3(2)	0.1150	1744.259	117.872	5

Ni-N(2.0) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	3(1)					
2Br	2.44(3)	14(3)	3(2)	0.1132	1717.045	116.033	5

Ni-N(2.0) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	3(1)					
2Br	3.30(0.16)	22(22)	4(2)	0.1327	2011.759	135.949	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.62(2)	2(2)					
1S	2.38(3)	4(3)	4(2)	0.0667	1010.788	78.981	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.37(3)	4(3)					
1S	2.63(2)	2(2)	4(2)	0.0591	896.705	70.067	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.37(3)	4(3)					
1S	2.63(2)	3(2)	4(2)	0.0569	862.477	67.392	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	1(1)					
1S	2.37(3)	4(3)					
1S	2.63(2)	3(2)	4(2)	0.0550	833.894	65.159	7

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.63(2)	2(2)					
1S	2.38(3)	4(3)	4(2)	0.0640	970.744	75.852	7

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.37(3)	4(3)					
1S	2.63(2)	2(2)	4(2)	0.0579	877.254	68.547	7

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.37(3)	4(3)					
1S	2.63(2)	2(2)	4(2)	0.0559	848.120	66.270	7

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.38(3)	4(3)					
1S	2.63(2)	2(2)	4(2)	0.0588	891.746	69.679	7

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.38(3)	4(3)					
1S	2.63(2)	2(2)	4(2)	0.0669	862.219	67.372	7

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.38(3)	4(3)					
1S	2.63(2)	2(2)	4(2)	0.0577	874.283	68.315	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.64(2)	1(1)					
1S	2.42(4)	7(4)	4(1)	0.0517	784.080	61.267	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.40(3)	6(3)					
1S	2.64(2)	2(2)	4(1)	0.0459	695.261	54.326	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.39(3)	6(3)					
1S	2.65(2)	2(2)	4(1)	0.0446	676.453	52.857	7

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O							
1S							
1S			No Fit	No Fit	No Fit	No Fit	7

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.40(3)	7(4)					
1S	2.65(2)	1(1)	4(1)	0.0457	692.676	54.124	7

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.40(3)	7(3)					
1S	2.65(2)	2(1)	4(1)	0.0444	673.825	52.651	7

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.41(3)	7(4)					
1S	2.65(2)	1(1)	4(1)	0.0456	691.705	54.049	7

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.41(3)	7(4)					
1S	2.65(2)	1(1)	4(1)	0.0444	672.915	52.580	7

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.65(2)	1(1)					
1S	2.42(3)	7(4)	4(1)	0.0457	692.679	54.125	7

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
1Br	2.42(4)	4(3)					
1Br	2.22(7)	6(5)	4(2)	0.0955	1448.241	113.163	7

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
1Br	2.20(7)	6(5)					
1Br	2.42(3)	4(3)	4(2)	0.0933	1415.340	110.592	7

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
1Br	2.43(3)	4(2)					
1Br	2.23(7)	7(6)	4(2)	0.0941	1427.269	111.524	7

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
1Br	2.21(7)	7(5)					
1Br	2.42(3)	4(3)	4(2)	0.0926	1404.646	109.756	7

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1Br	2.46(3)	8(3)					
1Br	2.77(4)	10(6)	3(2)	0.0974	1476.238	115.350	7

Ni-N(2.0) Ni-Br(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(2)	0(1)					
1Br	2.21(7)	7(5)					
1Br	2.43(3)	4(2)	4(2)	0.0912	1382.243	108.006	7

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	1(1)					
1Br	2.43(3)	3(2)					
1Br	2.25(5)	5(3)	5(2)	0.0676	1024.554	80.057	7

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	1(1)					
1Br	2.23(5)	5(3)					
1Br	2.43(3)	4(2)	5(2)	0.0651	986.922	77.116	7

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	2(1)					
1Br	2.44(3)	3(2)					
1Br	2.26(5)	5(3)	5(2)	0.0667	1011.500	79.037	7

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	1(1)					
1Br	2.24(5)	6(3)					
1Br	2.43(2)	4(2)	5(2)	0.0647	981.376	76.683	7

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	3(1)					
1Br	2.46(3)	10(4)					
1Br	2.77(3)	8(4)	3(2)	0.0725	1100.056	85.956	7

Ni-N(2.0) Ni-Br(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	1(1)					
1Br	2.24(5)	6(3)					
1Br	2.44(2)	4(2)	5(2)	0.0636	964.083	75.332	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	5(1)	3(1)	0.0433	656.085	51.265	7

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	1(0)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	6(1)	5(1)	0.0295	447.931	35.000	7

Ni-N(2.2) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	1(1)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	5(1)	3(1)	0.0344	522.129	40.798	7

Ni-N(2.0) Ni-N(2.2) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	3(1)					
1N/O	2.16(3)	4(4)					
1S	2.50(2)	8(2)					
1Br	2.45(2)	4(2)	5(1)	0.0346	448.509	41.537	9
2N/O	2.03(3)	3(2)					
2N/O	2.13(3)	3(4)					
1S	2.50(2)	8(2)					
1Br	2.45(2)	4(2)	5(1)	0.0361	547.429	50.698	9
1N/O	2.02(6)	4(3)					
3N/O	2.11(2)	1(4)					
1S	2.51(2)	8(2)					
1Br	2.45(2)	4(2)	4(1)	0.0384	581.828	53.884	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.3) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(2)	2(2)					
1N/O	2.15(5)	3(6)					
1S	2.50(2)	9(2)					
1Br	2.45(2)	5(2)	4(1)	0.0319	484.324	44.854	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.4) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(2)	2(2)					
1N/O	2.13(7)	3(7)					
1S	2.50(1)	9(2)					
1Br	2.44(1)	5(2)	4(1)	0.0302	457.291	42.350	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	2(2)					
1N/O	2.15(4)	4(4)					
1S	2.50(1)	9(2)					
1Br	2.45(1)	5(2)	4(1)	0.0282	427.835	39.622	9
2N/O	2.03(3)	3(2)					
2N/O	2.12(3)	2(5)					
1S	2.50(2)	9(2)					
1Br	2.45(1)	5(2)	4(1)	0.0295	446.675	41.367	9
1N/O	2.03(7)	4(3)					
3N/O	2.10(3)	1(4)					
1S	2.50(2)	9(2)					
1Br	2.45(1)	5(2)	4(1)	0.0312	472.537	43.762	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(1)	4(2)					
1N/O	1.99(2)	6(2)					
1S	2.51(2)	8(2)					
1Br	2.46(2)	4(2)	4(1)	0.0315	478.092	44.277	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.5) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(2)	2(2)					
1N/O	2.14(4)	4(5)					
1S	2.50(1)	5(2)					
1Br	2.45(2)	9(2)	4(1)	0.0290	440.027	40.751	9

Ni-N(2.0) Ni-N(2.2) Ni-S(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	3(1)					
1N/O	2.16(3)	5(4)					
1S	2.50(2)	8(2)					
1Br	2.45(2)	5(2)	5(1)	0.0302	458.323	42.446	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(2)	8(1)					
1Br	2.46(1)	4(1)	5(1)	0.0353	535.054	41.808	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(1)	7(1)					
1Br	2.47(1)	4(1)	5(1)	0.0336	508.907	39.765	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.52(2)	7(1)					
1Br	2.47(1)	3(1)	5(1)	0.0339	514.648	40.214	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	3(1)					
1S	2.33(3)	7(4)					
1Br	2.77(2)	6(2)	1(2)	0.0589	893.412	69.810	7

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(2)	8(1)					
1Br	2.46(1)	4(1)	4(1)	0.0354	537.085	41.967	7

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(1)	8(1)					
1Br	2.46(1)	4(1)	5(1)	0.0323	489.428	38.243	7

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(1)	8(1)					
1Br	2.47(1)	4(1)	5(1)	0.0317	481.163	37.597	7

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.06(2)	3(1)					
1S	2.31(4)	5(4)					
1Br	3.16(7)	11(8)	0(3)	0.1142	1731.291	135.280	7

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	1(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0359	545.070	42.591	7

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	1(1)					
1S	2.51(1)	8(1)					
1Br	2.46(1)	4(1)	4(1)	0.0319	483.602	37.788	7

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(1)	8(1)					
1Br	2.46(1)	4(1)	4(1)	0.0307	464.759	36.315	7

Ni-N(2.2) Ni-S(2.4) Ni-Br(2.5)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.08(1)	1(1)					
1S	2.51(2)	7(2)					
1Br	2.46(2)	4(2)	3(1)	0.0380	576.083	45.014	7

Ni-N(2.0) Ni-N(2.2) Ni-S(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1N/O	2.14(0.20)	17(20)					
1S	2.51(1)	9(1)					
1Br	2.46(1)	5(1)	4(2)	0.0294	446.050	41.309	9
3N/O	2.07(1)	2(1)					
2N/O	2.10(6)	9(7)					
1S	2.51(1)	9(2)					
1Br	2.46(1)	5(1)	4(1)	0.0300	454.929	42.131	9
2N/O	2.06(1)	3(2)					
3N/O	2.09(4)	6(4)					
1S	2.50(1)	9(2)					
1Br	2.45(1)	5(2)	4(1)	0.0309	469.295	43.462	9
1N/O	2.06(2)	5(2)					
4N/O	2.09(2)	4(2)					
1S	2.50(1)	9(2)					
1Br	2.45(1)	5(2)	3(1)	0.0324	491.270	45.497	9

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.07(1)	1(1)					
1S	2.64(2)	2(2)					
1Br	2.15(3)	7(3)	4(2)	0.0636	964.972	75.401	7

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.07(1)	1(1)					
1S	2.50(2)	8(1)					
1Br	2.44(1)	4(1)	4(1)	0.0382	579.201	45.258	7

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
5N/O	2.07(1)	1(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0337	510.413	39.883	7

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	1(1)					
1S	2.51(1)	8(1)					
1Br	2.46(1)	4(1)	4(1)	0.0319	483.350	37.768	7

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(1)	8(1)					
1Br	2.46(1)	4(1)	4(1)	0.0314	476.721	37.250	7

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.54(5)	0(6)					
1Br	2.47(4)	2(3)	4(2)	0.0476	722.303	56.439	7

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	1(1)					
1S	2.50(2)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0358	542.206	42.367	7

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	1(1)					
1S	2.51(1)	7(1)					
1Br	2.46(1)	4(1)	4(1)	0.0332	503.255	39.323	7

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	1(1)					
1S	2.51(1)	7(1)					
1Br	2.46(1)	4(1)	4(1)	0.0323	489.914	38.281	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.7)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(1)	1(1)					
1S	2.43(8)	0(7)					
1Br	2.41(6)	2(4)	4(3)	0.0929	1408.172	110.032	7
2N/O	2.05(2)	2(1)	1(4)	0.1139	1727.326	134.970	7

2S	2.36(6)	5(6)					
1Br	2.37(6)	5(4)					
1N/O	2.02(2)	4(2)					
3S	2.29(7)	5(4)					
1Br	2.29(0.10)	5(7)	neg4(6)	0.1348	2043.901	159.707	7
2N/O	2.06(2)	2(1)					
1S	2.38(8)	1(5)					
2Br	2.38(6)	8(6)	3(4)	0.1475	2236.908	174.788	7
1N/O	2.02(4)	5(2)					
1S	2.27(5)	0(3)					
3Br	1.94(9)	20(9)	neg6(7)	0.2011	3049.450	238.278	7

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	3(1)					
1S	2.37(5)	11(8)					
1S	2.49(1)	10(1)					
1Br	2.44(1)	6(1)	4(2)	0.0387	586.599	54.325	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	3(1)					
1S	2.36(4)	8(6)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	6(1)	4(2)	0.0367	555.773	51.471	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	2(1)					
1S	2.36(3)	6(5)					
1S	2.49(2)	9(1)					
1Br	2.45(2)	5(1)	3(2)	0.0363	551.015	51.030	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	0(1)					
1S	2.31(3)	3(2)					
1S	1.75(0.10)	24(11)					
1Br	2.78(2)	7(2)	1(3)	0.0662	1003.653	92.949	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	3(1)					
1S	2.37(7)	14(10)					
1S	2.49(1)	10(1)					
1Br	2.44(1)	6(1)	3(2)	0.0368	557.548	51.635	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	3(1)					
1S	2.35(4)	10(7)					
1S	2.49(1)	10(1)					
1Br	2.44(1)	6(1)	3(2)	0.0349	529.818	49.067	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(1)	1(1)					
1S	2.37(0.44)	5(155)					
1S	2.52(0.91)	7(198)					
1Br	2.43(0.79)	5(57)	3(3)	0.0694	1052.112	97.437	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	1(1)					
1S	2.37(0.36)	5(144)					
1S	2.52(0.83)	7(185)					
1Br	2.43(0.73)	5(67)	3(3)	0.0685	1038.839	96.208	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)					
1S	2.38(0.75)	4(125)					
1S	2.54(0.80)	8(223)					
1Br	2.42(0.86)	5(50)	3(3)	0.0710	1076.904	99.733	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	2(1)					
1S	2.34(5)	11(8)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	6(1)	3(2)	0.0367	556.928	51.578	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	2(1)					
1S	2.34(4)	8(6)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	3(2)	0.0360	546.193	50.583	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	1(1)					
1S	2.37(0.35)	5(124)					
1S	2.53(0.73)	7(180)					
1Br	2.43(0.77)	5(57)	3(3)	0.0675	1023.086	94.749	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)					
1S	2.38(0.73)	4(111)					
1S	2.55(0.67)	8(235)					
1Br	2.42(0.97)	6(51)	3(3)	0.0699	1060.367	98.202	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)					
1S	2.37(0.53)	4(116)					
1S	2.54(0.65)	8(212)					
1Br	2.42(0.94)	6(43)	3(3)	0.0685	1038.810	96.205	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	2(1)					
1S	2.33(4)	9(7)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	3(2)	0.0388	588.996	54.548	9

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	1(1)					
1S	2.37(0.34)	5(106)					
1S	2.53(0.62)	7(173)					
1Br	2.43(0.79)	6(50)	3(3)	0.0666	1009.710	93.510	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	3(1)					
1S	2.38(7)	16(11)					
1S	2.49(1)	10(1)					
1Br	2.44(1)	6(1)	3(2)	0.0374	566.423	52.457	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	3(1)					
1S	2.36(5)	10(7)					
1S	2.49(1)	10(1)					
1Br	2.44(1)	6(1)	3(2)	0.0357	541.711	50.168	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	2(1)					
1S	2.36(4)	8(6)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	3(2)	0.0353	536.019	49.641	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	1(1)					
1S	2.31(2)	1(2)					
1S	2.50(4)	3(4)					
1Br	2.79(2)	4(2)	1(2)	0.0471	713.472	66.075	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(2)					
1S	2.39(0.86)	4(135)					
1S	2.54(0.89)	9(201)					
1Br	2.42(0.70)	5(48)	3(3)	0.0716	1086.200	100.594	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	3(1)					
1S	2.35(5)	12(8)					
1S	2.49(1)	10(1)					
1Br	2.44(1)	6(1)	3(2)	0.0376	570.088	52.796	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	2(1)					
1S	2.35(4)	9(6)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	3(2)	0.0370	560.463	51.905	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(2)					
1S	2.39(0.78)	4(128)					
1S	2.55(0.80)	9(190)					
1Br	2.42(0.76)	5(52)	3(4)	0.0705	1069.916	99.059	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)					
1S	2.39(0.95)	4(143)					
1S	2.55(1.0)	9(246)					
1Br	2.42(0.82)	5(60)	3(3)	0.0692	1048.985	97.148	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.06(1)	2(1)					
1S	2.34(5)	10(7)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	2(2)	0.0400	606.086	56.130	9

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(1)					
1S	2.38(0.63)	5(139)					
1S	2.54(0.93)	9(224)					
1Br	2.42(0.86)	5(49)	3(3)	0.0674	1021.868	94.636	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(2)					
1S	2.40(0.60)	4(125)					
1S	2.55(0.78)	10(147)					
1Br	2.42(0.63)	5(27)	3(3)	0.0721	1093.020	101.226	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(2)					
1S	2.40(0.56)	4(125)					
1S	2.56(0.74)	9(136)					
1Br	2.42(0.70)	5(30)	3(3)	0.0710	1076.413	99.688	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(2)					
1S	2.40(0.80)	4(148)					
1S	2.55(0.99)	10(184)					
1Br	2.42(0.72)	5(43)	3(4)	0.0697	1056.621	97.855	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(2)					
1S	2.41(0.45)	4(126)					
1S	2.56(0.75)	10(118)					
1Br	2.42(0.68)	5(21)	3(3)	0.0714	1082.676	100.268	9

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(2)	1(2)					
1S	2.40(0.62)	4(143)					
1S	2.55(0.93)	10(149)					
1Br	2.42(0.69)	5(27)	3(3)	0.0701	1063.555	98.497	9

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O							
1S							
1S							
1Br			No Fit	No Fit	No Fit	No Fit	9

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	1(2)					
1S	3.08(6)	8(8)					
1S	1.85(4)	13(5)					
1Br	2.46(2)	7(2)	7(2)	0.0745	1129.445	104.599	9

Table K.3. Additional Fits for Ni(II) C201A-PHD2 in Buffer with 50 mM PBS, 150 mM NaBr at pH 7.2.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 2.5 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(4)	0(3)	7(9)	0.3953	8231.823	1211.119	3
3N/O	2.10(3)	2(2)	6(6)	0.2708	5015.489	737.911	3
4N/O	2.10(2)	3(2)	6(4)	0.1928	3569.929	525.231	3
5N/O	2.10(2)	4(2)	6(3)	0.1473	2728.865	401.488	3
6N/O	2.10(2)	6(2)	5(3)	0.1257	2328.218	342.542	3
7N/O	2.10(2)	7(2)	5(2)	0.1217	2253.145	331.497	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.20(4)	4(2)	neg13(10)	0.3223	5968.594	878.138	3
3S	2.20(3)	6(2)	neg14(7)	0.2320	4297.347	632.253	3
4S	2.20(3)	8(2)	neg14(6)	0.1851	3428.713	504.454	3
5S	2.20(3)	9(2)	neg15(5)	0.1632	3022.440	444.681	3
6S	2.20(3)	11(2)	neg15(5)	0.1563	2895.510	426.006	3
7S	2.20(3)	12(2)	neg15(5)	0.1588	2940.370	432.606	3

Ni-N(2.0) Ni-N(2.2)

N	Radius Å	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.05(2)	5(2)					
1N/O	2.18(2)	8(2)	5(4)	0.1344	2488.599	518.796	5
2N/O	2.03(2)	4(2)					
2N/O	2.16(2)	5(2)	4(3)	0.0879	1627.059	339.192	5
3N/O	2.06(2)	2(1)					
1N/O	2.19(2)	7(2)	5(3)	0.0916	1697.004	353.773	5
4N/O	2.06(2)	0(1)					
1N/O	2.19(2)	6(2)	4(3)	0.0786	1454.961	303.314	5
3N/O	2.04(2)	2(2)					
2N/O	2.17(2)	4(2)	4(3)	0.0783	1450.385	302.360	5
5N/O	2.07(2)	2(2)					
1N/O	2.19(2)	5(2)	4(3)	0.0846	1566.195	326.503	5
4N/O	2.05(2)	1(2)					
2N/O	2.18(2)	3(2)	4(3)	0.0877	1623.515	338.453	5
3N/O	2.02(2)	1(2)					
3N/O	2.16(2)	1(2)	3(3)	0.0900	1667.101	347.539	5

6N/O	2.07(2)	4(2)					
1N/O	2.19(3)	3(3)	3(3)	0.1025	1898.905	395.863	5
5N/O	2.05(3)	3(3)					
2N/O	2.18(3)	1(3)	3(3)	0.1082	2004.780	417.935	5
4N/O	2.03(3)	2(3)					
3N/O	2.17(3)	0(3)	3(3)	0.1122	2078.863	433.379	5

Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.14(4)	0(2)					
1S	2.27(4)	3(2)	neg16(7)	0.1620	2999.758	625.357	5
2S	2.12(4)	1(2)					
2S	2.26(4)	1(3)	neg16(6)	0.1467	2716.693	566.346	5
3S	2.15(4)	3(2)					
1S	2.28(4)	1(3)	neg16(7)	0.1480	2741.089	571.432	5
4S	2.16(4)	6(3)					
1S	2.29(5)	1(4)	neg16(7)	0.1486	2753.070	573.930	5
3S	2.14(4)	4(3)					
2S	2.27(5)	2(4)	neg16(7)	0.1484	2748.066	572.887	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.20(5)	8(5)					
2S	2.30(0.32)	16(42)	neg13(10)	0.1544	2859.000	596.013	5
3S	2.23(0.51)	12(54)					
3S	2.18(0.42)	9(13)	neg15(10)	0.1560	2889.741	602.422	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.22(4)	9(3)					
2S	2.42(0.13)	15(23)	neg10(7)	0.1417	2624.473	547.121	5
4S	2.21(3)	8(3)					
3S	2.36(0.16)	20(29)	neg10(8)	0.1451	2687.064	560.170	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.01(3)	2(2)					
1S	2.27(3)	1(2)	neg4(6)	0.1552	2874.495	599.243	5

1N/O	1.98(4)	3(2)					
2S	2.24(3)	2(2)	neg8(7)	0.1615	2990.186	623.361	5
2N/O	2.00(4)	0(3)					
2S	2.26(4)	3(2)	neg7(6)	0.1441	2668.786	556.359	5
3N/O	2.03(3)	1(2)					
1S	2.28(3)	0(2)	neg3(5)	0.1301	2408.655	502.130	5
1N/O	1.97(4)	2(3)					
3S	2.23(4)	5(2)	neg10(6)	0.1480	2741.619	571.543	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.04(3)	3(2)					
1S	2.29(3)	1(3)	neg2(5)	0.1211	2242.624	467.518	5
2N/O	1.99(6)	2(4)					
3S	2.25(4)	6(3)	neg8(7)	0.1471	2723.555	567.777	5
3N/O	2.01(5)	3(3)					
2S	2.27(4)	4(3)	neg5(6)	0.1399	2591.142	540.173	5
5N/O	2.05(4)	5(3)					
1S	2.29(4)	2(4)	neg1(5)	0.1206	2234.262	465.774	5
1N/O	1.99(9)	2(8)					
5S	2.23(5)	10(3)	neg12(7)	0.1520	2815.838	587.015	5
4N/O	2.03(6)	5(4)					
2S	2.27(5)	6(4)	neg4(7)	0.1398	2589.292	539.787	5
2N/O	2.00(8)	4(7)					
4S	2.24(5)	9(3)	neg9(7)	0.1520	2814.728	586.784	5
3N/O	2.02(7)	5(5)					
3S	2.25(5)	8(4)	neg7(7)	0.1487	2753.865	574.096	5
6N/O	2.08(5)	7(3)					
1S	2.28(5)	5(7)	1(5)	0.1221	2260.957	471.340	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.06(7)	7(4)					
2S	2.27(5)	8(7)	neg2(7)	0.1391	2576.225	537.063	5
2N/O			No Fit	No Fit	No Fit	No Fit	5

5S							
4N/O	2.04(7)	7(6)					
3S	2.25(6)	9(6)	neg5(8)	0.1491	2761.184	575.621	5
3N/O	2.03(8)	7(9)					
4S	2.24(6)	10(5)	neg8(8)	0.1537	2845.786	593.258	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.07(5)	0(3)					5
1Br	2.42(6)	5(3)	3(10)	0.2663	4931.634	1028.093	
1N/O	2.06(8)	3(4)					5
2Br	2.41(0.10)	8(4)	1(20)	0.4335	8028.989	1673.796	
2N/O	2.08(5)	0(3)					
2Br	2.43(7)	10(5)	4(11)	0.2936	5438.139	1133.684	5
3N/O	2.08(4)	2(2)					
1Br	2.42(4)	6(3)	4(7)	0.1778	3293.338	686.559	5
1N/O	1.91(8)	1(5)					
3Br	2.27(8)	8(3)	neg35(20)	0.3488	6459.421	1346.589	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.09(3)	3(2)					
1Br	2.42(4)	7(3)	4(5)	0.1225	2268.041	472.816	5
2N/O	2.09(5)	1(4)					
3Br	2.43(7)	14(6)	5(11)	0.3127	5791.240	1207.294	5
3N/O	2.09(4)	2(3)					
2Br	2.43(5)	11(5)	5(7)	0.2011	3724.539	776.451	5
5N/O	2.10(3)	5(2)					
1Br	2.42(3)	7(3)	5(3)	0.0887	1642.141	342.336	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.10(3)	4(2)					
2Br	2.42(4)	12(5)	6(5)	0.1382	2559.728	533.624	5
2N/O	2.10(5)	1(4)					
4Br	2.44(8)	17(7)	6(10)	0.3260	6038.220	1258.782	5
3N/O	2.11(4)	2(3)	6(6)	0.2142	3966.784	826.952	5

3Br	2.43(6)	15(6)					
6N/O	2.10(2)	7(2)					
1Br	2.41(3)	8(3)	5(3)	0.0701	1298.502	270.697	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.11(3)	5(2)					
2Br	2.41(4)	13(5)	6(3)	0.0969	1794.072	374.008	5
2N/O	2.11(5)	1(4)					
5Br	2.44(8)	19(8)	7(10)	0.3363	6228.213	1298.390	5
4N/O	2.11(3)	4(3)					
3Br	2.42(5)	16(6)	6(4)	0.1462	2708.202	564.576	5
3N/O	2.11(4)	2(3)					
4Br	2.43(6)	18(7)	7(6)	0.2233	4136.032	862.235	5

Table K.4. Additional Fits for Ni(II) C201A-PHD2 in Buffer with 50 mM Hepes, 150 mM NaBr at pH 7.2.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(3)	0(2)	7(6)	0.4089	7845.846	467.074	3
3N/O	2.10(2)	2(1)	7(4)	0.2876	5518.577	328.529	3
4N/O	2.10(2)	3(1)	6(3)	0.2119	4065.009	241.996	3
5N/O	2.10(1)	4(1)	6(2)	0.1681	3224.979	191.988	3
6N/O	2.10(1)	6(1)	5(2)	0.1476	2831.391	168.557	3
7N/O	2.10(1)	7(1)	5(2)	0.1442	2767.120	164.731	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.20(3)	4(1)	neg13(7)	0.3380	6485.626	386.099	3
3S	2.20(2)	6(1)	neg14(5)	0.2505	4805.728	286.092	3
4S	2.20(2)	8(1)	neg14(4)	0.2052	3937.132	234.383	3
5S	2.20(2)	9(1)	neg15(4)	0.1842	3534.697	210.426	3
6S	2.20(2)	11(1)	neg15(3)	0.1779	3413.149	203.190	3
7S	2.20(2)	12(1)	neg15(3)	0.1805	3463.764	206.203	3

Ni-N(2.0) Ni-N(2.2)

N	Radius Å	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.05(2)	4(1)					
1N/O	2.18(2)	7(1)	5(3)	0.1734	3326.568	224.801	5

2N/O	2.03(1)	4(1)					
2N/O	2.16(1)	4(1)	4(2)	0.1233	2366.107	159.895	5
3N/O	2.06(1)	2(1)					
1N/O	2.18(1)	6(1)	5(2)	0.1274	2445.129	165.235	5
4N/O	2.06(1)	0(1)					
1N/O	2.19(1)	5(1)	4(2)	0.1113	2134.904	144.271	5
3N/O	2.04(1)	1(1)					
2N/O	2.17(1)	3(1)	4(2)	0.1102	2113.734	142.841	5
5N/O	2.07(1)	2(1)					
1N/O	2.19(2)	4(2)	4(2)	0.1143	2193.352	148.221	5
4N/O	2.05(1)	1(1)					
2N/O	2.18(2)	2(1)	4(2)	0.1163	2232.177	150.845	5
3N/O	2.03(2)	0(1)					
3N/O	2.16(1)	1(1)	3(2)	0.1181	2266.360	153.155	5
6N/O	2.07(2)	4(1)					
1N/O	2.19(2)	3(2)	3(2)	0.1295	2484.840	167.919	5
5N/O	2.05(2)	3(2)					
2N/O	2.18(2)	1(2)	3(2)	0.1341	2573.011	173.877	5
4N/O	2.04(2)	2(2)					
3N/O	2.16(2)	1(2)	3(2)	0.1375	2638.667	178.314	5

Ni-S(2.2) Ni-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.14(2)	1(1)					
1S	2.27(2)	2(1)	neg16(5)	0.1913	3669.811	247.996	5
2S	2.12(2)	2(2)					
2S	2.26(2)	1(2)	neg16(4)	0.1723	3306.287	223.430	5
3S	2.15(2)	4(1)					
1S	2.28(3)	1(2)	neg16(4)	0.1743	3343.452	225.942	5
4S	2.16(3)	6(2)					
1S	2.28(4)	1(3)	neg16(4)	0.1726	3311.263	223.766	5
3S	2.14(3)	5(2)					
2S	2.27(3)	3(2)	neg16(4)	0.1718	3296.728	222.784	5
5S	2.20(2)	9(1)	neg14(3)	0.1147	2200.538	148.707	5

1S	2.91(3)	3(3)					
4S	2.20(3)	8(3)					
2S	2.30(0.19)	16(26)	neg13(6)	0.1755	3367.460	227.564	5
3S	2.23(0.27)	12(27)					
3S	2.19(0.19)	9(7)	neg15(6)	0.1775	3404.922	230.096	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S	2.22(2)	9(2)					
2S	2.42(8)	15(14)	neg10(4)	0.1632	3131.165	211.596	5
4S	2.21(2)	8(2)					
3S	2.36(9)	20(17)	neg10(5)	0.1663	3190.899	215.633	5

Ni-N(2.0) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.01(2)	1(1)					5
1S	2.27(2)	1(1)	neg4(4)	0.1874	3596.311	243.029	
1N/O	1.98(3)	3(2)					5
2S	2.24(2)	2(1)	neg9(4)	0.1903	3650.890	246.718	
2N/O	2.00(3)	1(2)					
2S	2.25(2)	3(1)	neg7(4)	0.1706	3272.494	221.147	5
3N/O	2.03(2)	1(1)					
1S	2.28(2)	0(1)	neg3(4)	0.1591	3052.984	206.313	5
1N/O	1.97(3)	1(2)					
3S	2.23(2)	5(1)	neg10(4)	0.1735	3328.804	224.952	5
1N/O							
4S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.04(2)	3(1)					
1S	2.29(2)	1(2)	neg2(3)	0.1475	2829.282	191.195	5
2N/O	1.99(4)	2(2)					
3S	2.24(3)	6(2)	neg9(4)	0.1708	3277.388	221.477	5
3N/O	2.02(3)	3(2)					
2S	2.26(3)	4(2)	neg5(4)	0.1644	3153.695	213.118	5
5N/O	2.06(3)	5(2)					
1S	2.29(3)	3(2)	neg1(3)	0.1449	2780.537	187.901	5

1N/O	1.99(6)	3(5)					
5S	2.22(3)	10(2)	neg12(4)	0.1747	3352.517	226.554	5
4N/O	2.04(4)	6(2)					
2S	2.27(3)	6(3)	neg4(4)	0.1629	3125.406	211.207	5
2N/O	2.01(5)	5(4)					
4S	2.24(3)	9(2)	neg9(5)	0.1745	3348.839	226.306	5
3N/O	2.02(4)	5(3)					
3S	2.25(3)	8(2)	neg7(5)	0.1714	3288.632	222.237	5
6N/O	2.08(3)	7(2)					
1S	2.28(3)	5(4)	1(3)	0.1450	2781.791	187.986	5
1N/O							
6S			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.06(4)	7(3)					
2S	2.27(3)	8(4)	neg2(4)	0.1615	3099.158	209.433	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.05(5)	7(4)					
3S	2.25(4)	9(4)	neg5(5)	0.1713	3287.297	222.147	5
3N/O	2.03(5)	7(6)					
4S	2.24(4)	10(3)	neg8(5)	0.1758	3373.313	227.960	5

Ni-N(2.0) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.08(3)	0(2)					5
1Br	2.42(3)	5(2)	4(6)	0.2875	5515.955	372.754	
1N/O	2.06(4)	2(3)					5
2Br	2.42(5)	9(3)	2(11)	0.4487	8608.418	581.734	
2N/O	2.08(3)	0(2)					
2Br	2.43(4)	10(3)	5(6)	0.3089	5927.424	400.560	5
3N/O	2.08(2)	2(1)					
1Br	2.42(3)	6(2)	4(4)	0.1989	3816.032	257.877	5
1N/O	1.91(5)	1(3)					
3Br	2.27(4)	8(2)	neg35(12)	0.3664	7030.486	475.102	5
1N/O							
4Br			No Fit	No Fit	No Fit	No Fit	5

4N/O	2.09(2)	3(1)					
1Br	2.42(2)	7(2)	5(3)	0.1438	2759.925	186.508	5
2N/O	2.09(3)	1(2)					
3Br	2.43(4)	14(3)	5(6)	0.3264	6261.912	423.164	5
3N/O	2.10(2)	2(2)					
2Br	2.43(3)	11(3)	5(4)	0.2179	4181.365	282.566	5
5N/O	2.10(2)	5(1)					
1Br	2.42(2)	8(2)	5(2)	0.1108	2125.234	143.618	5
1N/O							
5Br			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.11(2)	4(1)					
2Br	2.42(3)	12(3)	6(3)	0.1568	3007.720	203.254	5
2N/O	2.10(3)	1(2)					
4Br	2.44(4)	16(4)	6(6)	0.3397	6516.858	440.392	5
3N/O	2.11(2)	2(2)					
3Br	2.43(3)	15(4)	6(4)	0.2303	4418.855	298.615	5
6N/O	2.10(1)	7(1)					
1Br	2.41(2)	8(2)	5(2)	0.0931	1786.569	120.732	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.11(2)	5(1)					
2Br	2.41(2)	13(3)	6(2)	0.1170	2244.596	151.684	5
2N/O	2.11(3)	1(2)					
5Br	2.44(5)	19(5)	7(6)	0.3504	6723.693	454.370	5
4N/O	2.11(2)	4(1)					
3Br	2.42(3)	12(3)	6(3)	0.1568	3007.720	203.254	5
3N/O	2.10(3)	1(2)					
4Br	2.44(4)	16(4)	6(6)	0.3397	6516.858	440.392	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.07(1)	2(1)					
1S	2.49(1)	10(1)					
1Br	2.44(1)	6(1)	5(2)	0.0658	1261.545	98.575	7
2N/O	2.03(2)	1(2)	neg1(4)	0.1228	2355.646	184.066	7

2S	2.35(5)	3(5)					
1Br	2.35(5)	3(3)					
1N/O							
3S							
1Br			No Fit	No Fit	No Fit	No Fit	7
2N/O	2.01(3)	2(2)					
1S	2.27(2)	1(2)					
2Br	2.17(0.19)	26(31)	neg4(4)	0.1758	3372.037	263.485	7
1N/O	1.98(3)	3(3)					
1S	2.25(3)	1(3)					
3Br	1.99(0.14)	24(15)	neg7(7)	0.2171	4164.525	325.408	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	5(1)	0.0390	749.179	58.539	7
3N/O	2.06(2)	1(1)					
2S	2.41(4)	7(5)					
1Br	2.39(3)	3(2)	2(3)	0.0892	1711.966	133.770	7
2N/O	2.03(2)	0(1)					
3S	2.36(4)	8(4)					
1Br	2.36(3)	3(2)	neg1(3)	0.1037	1990.151	155.507	7
1N/O							
4S							
1Br			No Fit	No Fit	No Fit	No Fit	7
3N/O	2.08(2)	2(1)					
1S	2.41(7)	1(5)					
2Br	2.39(5)	6(4)	4(3)	0.1204	2309.303	180.445	7
2N/O	2.12(3)	1(2)					
1S	1.12(0.13)	25(22)					
3Br	2.45(4)	15(4)	10(6)	0.2754	5284.412	412.914	7
1N/O							
1S							
4Br			No Fit	No Fit	No Fit	No Fit	7

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**

5N/O	2.08(1)	2(1)					
1S	2.49(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0357	770.818	60.230	7
4N/O	2.07(1)	3(1)					
2S	2.46(4)	10(5)					
1Br	2.42(2)	4(2)	4(2)	0.0661	1267.562	99.045	7
3N/O	2.06(2)	1(1)					
3S	2.42(4)	13(4)					
1Br	2.40(2)	4(1)	2(2)	0.0760	1458.500	113.964	7
2N/O	2.03(2)	0(1)					
4S	2.37(3)	13(4)					
1Br	2.37(2)	4(1)	0(3)	0.0913	1751.840	136.885	7
4N/O	2.08(2)	4(1)					
1S	2.43(6)	0(5)					
2Br	2.40(4)	6(4)	4(2)	0.0838	1608.776	125.707	7
3N/O	2.07(3)	1(2)					
1S	2.33(4)	1(2)					
3Br	2.33(5)	13(5)	2(3)	0.1219	2339.013	182.766	7
2N/O							
1S							
4Br			No Fit	No Fit	No Fit	No Fit	7
3N/O	2.06(1)	2(1)					
2S	2.42(4)	2(4)					
2Br	2.39(3)	4(3)	3(2)	0.0719	1378.598	107.721	7
2N/O	2.03(2)	0(1)					
3S	2.37(3)	5(3)					
2Br	2.36(3)	5(2)	0(3)	0.0819	1572.201	122.849	7
2N/O	2.06(2)	1(1)					
2S	2.38(5)	2(3)					
3Br	2.36(4)	8(3)	2(3)	0.1160	2224.811	173.843	7
1N/O	2.03(2)	2(1)					
3S	2.34(5)	3(3)					
3Br	2.32(5)	7(3)	neg2(4)	0.1191	2284.980	178.544	7

Ni-N(2.0) Ni-S(2.2)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
6N/O	2.08(3)	7(2)					
1S	2.28(3)	5(4)	1(3)	0.1450	2781.791	187.986	5

Ni-N(2.0) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.08(3)	7(2)					
1S	2.28(3)	5(4)	1(4)	0.1477	2833.194	191.460	5

Ni-N(2.0) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.07(3)	7(2)					
1S	2.28(3)	5(4)	0(4)	0.1501	2880.251	194.640	5

Ni-N(2.0) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.11(1)	5(1)					
1S	2.64(2)	3(2)	6(1)	0.0662	1269.238	85.772	5

Ni-N(2.0) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.11(1)	5(1)					
1S	2.64(2)	3(2)	6(1)	0.0654	1255.411	84.837	5

Ni-N(2.0) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.10(1)	7(1)					
1Br	2.41(2)	8(2)	5(2)	0.0931	2008.710	135.743	5

Ni-N(2.0) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.10(1)	6(1)					
1Br	2.41(2)	8(2)	5(2)	0.0905	1736.483	117.347	5

Ni-N(2.0) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.10(1)	6(1)					
1Br	2.41(2)	8(2)	5(2)	0.0884	1695.578	114.583	5

Ni-N(2.0) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
6N/O	2.10(1)	6(1)					
1Br	3.35(0.10)	13(12)	5(2)	0.1383	2653.944	179.347	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.06(4)	7(3)					
2S	2.27(3)	8(4)	neg2(4)	0.1615	3099.158	209.433	5

Ni-N(2.0) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.06(4)	7(3)					
2S	2.27(3)	8(4)	neg3(5)	0.1656	3177.460	214.724	5

Ni-N(2.0) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(1)	4(1)					
2S	2.65(2)	8(2)	7(1)	0.0992	1902.880	128.592	5

Ni-N(2.0) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(1)	4(1)					
2S	2.65(2)	8(2)	7(1)	0.0976	1872.875	126.564	5

Ni-N(2.0) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(1)	4(1)					
2S	2.66(2)	9(3)	7(1)	0.0969	1859.717	125.675	5

Ni-N(2.0) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	5N/O	2.11(2)	5(1)				
2Br	2Br	2.41(2)	13(3)	6(2)	0.1170	2244.596	5

Ni-N(2.0) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(2)	5(1)					
2Br	2.41(2)	13(3)	6(2)	0.1137	2181.217	147.401	5

Ni-N(2.0) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(2)	5(1)					
2Br	2.42(2)	13(3)	6(2)	0.1109	2127.127	143.746	5

Ni-N(2.0) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

5N/O	2.10(1)	4(1)					
2Br	3.36(9)	17(11)	6(2)	0.1543	2961.072	200.101	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.58(3)	3(3)					
1S	2.34(3)	3(3)	3(2)	0.0893	1713.582	133.896	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.33(3)	3(3)					
1S	2.59(3)	3(3)	3(2)	0.0786	1508.094	117.840	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.33(2)	3(2)					
1S	2.59(3)	3(3)	3(2)	0.0760	1458.567	113.970	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	3(1)					
1S	2.33(2)	3(2)					
1S	2.60(3)	4(3)	3(2)	0.0742	1423.129	111.201	5

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.34(3)	3(3)					
1S	2.59(3)	3(3)	3(2)	0.0812	1557.291	121.684	5

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.34(3)	3(3)					
1S	2.59(3)	3(3)	3(2)	0.0785	1506.378	117.706	5

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)	3(2)	0.0766	1470.002	114.863	5

1S	2.33(2)	3(2)					
1S	2.59(3)	3(3)					

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.34(3)	3(3)					
1S	2.59(3)	3(3)	3(2)	0.0808	1549.968	121.112	5

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.34(3)	3(3)					
1S	2.59(3)	3(3)	3(2)	0.0788	1512.796	118.207	5

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(2)	3(1)					
1S	2.34(3)	3(3)					
1S	2.59(3)	3(3)	2(2)	0.0808	1550.084	121.121	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.10(2)	4(1)					
1S	3.02(5)	3(6)					
1S	3.19(6)	3(7)	4(2)	0.1337	2565.871	200.492	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(1)	4(1)					
1S	2.36(4)	7(4)					
1S	2.61(2)	2(2)	4(2)	0.0648	1242.602	97.095	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	4(1)					
1S	2.35(3)	6(4)					
1S	2.61(2)	2(2)	4(2)	0.0629	1206.849	94.301	5

Ni-N(2.0) Ni-S(2.2) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	4(1)	4(2)	0.0617	1183.617	92.486	5

1S	2.35(3)	6(4)					
1S	2.61(2)	3(2)					

Ni-N(2.0) Ni-S(2.3) Ni-S(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.12(2)	7(3)					
1S	1.90(4)	10(6)					
1S	1.13(9)	38(29)	10(3)	0.1183	2268.847	177.283	5

Ni-N(2.0) Ni-S(2.3) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(1)	4(1)					
1S	2.36(4)	7(5)					
1S	2.61(2)	2(2)	4(2)	0.0642	1231.779	96.249	5

Ni-N(2.0) Ni-S(2.3) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	4(1)					
1S	2.35(3)	7(4)					
1S	2.61(2)	3(2)	4(2)	0.0630	1208.458	94.427	5

Ni-N(2.0) Ni-S(2.4) Ni-S(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(1)	4(1)					
1S	2.36(4)	7(5)					
1S	2.62(2)	2(2)	4(2)	0.0654	1254.294	98.008	5

Ni-N(2.0) Ni-S(2.4) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	4(1)					
1S	2.36(4)	7(5)					
1S	2.62(2)	2(2)	4(2)	0.0642	1231.179	96.202	5

Ni-N(2.0) Ni-S(2.5) Ni-S(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(2)	6(2)					
1S	1.88(7)	13(7)					
1S	1.85(0.60)	62(146)	8(3)	0.1223	2346.253	183.332	5

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(3)	0(2)	3(3)	0.1192	2287.079	178.708	5

1Br	2.37(4)	4(3)					
1Br	2.16(5)	3(4)					

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(3)	1(2)					
1Br	2.14(5)	3(4)					
1Br	2.37(4)	5(3)	3(3)	0.1154	2213.363	172.948	5

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O							
1Br							
1Br			No Fit	No Fit	No Fit	No Fit	5

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(3)	0(2)					
1Br	2.38(4)	4(3)					
1Br	2.17(5)	4(4)	3(3)	0.1175	2253.610	176.093	5

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.09(2)	3(1)					
1Br	2.43(3)	7(3)					
1Br	2.77(0.11)	15(14)	5(3)	0.1352	2593.461	202.648	5

Ni-N(2.0) Ni-Br(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.17(1)	0(1)					
1Br	2.82(3)	9(4)					
1Br	1.97(1)	4(1)	10(2)	0.0867	1662.567	129.910	5

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	2(2)					
1Br	2.21(6)	6(4)					
1Br	2.41(3)	4(2)	5(2)	0.0853	1637.276	127.934	5

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.09(2)	2(2)	5(2)	0.0840	1612.616	126.007	5

1Br	2.21(6)	6(4)					
1Br	2.41(3)	4(2)					

Ni-N(2.0) Ni-Br(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.10(2)	5(1)					
1Br	2.42(2)	8(2)					
1Br	3.36(9)	13(10)	5(2)	0.1023	1963.569	153.430	5

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.10(2)	3(2)					
1Br	2.41(3)	4(2)					
1Br	2.23(6)	7(4)	5(2)	0.0852	1633.816	127.663	5

Ni-N(2.0) Ni-Br(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.10(2)	5(1)					
1Br	2.42(3)	9(3)					
1Br	2.79(8)	14(9)	5(2)	0.0996	1910.659	149.295	5

Ni-N(2.0) Ni-Br(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.16(1)	2(1)					
1Br	2.81(3)	9(3)					
1Br	1.96(1)	5(1)	9(1)	0.0695	1334.322	104.261	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	1(1)					
1S	2.49(1)	8(1)					
1Br	2.44(1)	5(1)	3(1)	0.0446	856.143	66.897	5

Ni-N(2.0) Ni-N(2.2) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.05(1)	2(1)					
1N/O	2.17(3)	4(4)					
1S	2.48(2)	8(2)					
1Br	2.43(2)	4(2)	5(1)	0.0343	658.137	60.951	9
2N/O	2.03(2)	3(2)					
2N/O	2.14(2)	2(4)					
1S	2.48(2)	8(2)	4(1)	0.0351	672.583	62.289	9

1Br	2.43(2)	4(2)					
1N/O	2.00(4)	4(2)					
3N/O	2.11(2)	0(3)					
1S	2.48(2)	8(2)					
1Br	2.43(2)	4(2)	4(1)	0.0367	703.281	65.132	9

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	5(1)	5(1)	0.0408	783.158	61.194	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.08(1)	1(1)					
1S	2.50(1)	8(1)					
1Br	2.46(1)	4(1)	5(1)	0.0436	836.427	65.357	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.04(2)	3(1)					
1S	2.29(2)	1(2)					
1Br	2.75(3)	9(3)	neg2(3)	0.1054	2022.690	158.049	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	4(1)	0.0353	678.078	52.984	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	5(1)	5(1)	0.0352	675.318	52.768	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	5(1)	5(1)	0.0367	703.913	55.002	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.04(2)	3(1)					
1S	2.29(2)	2(2)					
1Br	2.75(3)	9(3)	neg2(3)	0.1085	2081.953	162.680	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	6(1)	4(1)	0.0348	667.891	52.188	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.50(1)	9(1)					
1Br	2.44(1)	5(1)	4(1)	0.0333	638.648	49.903	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	5(1)	4(1)	0.0335	642.969	50.240	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.04(2)	3(1)					
1S	2.29(2)	2(2)					
1Br	2.74(3)	9(4)	neg3(3)	0.1111	2131.215	166.529	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	0(1)					
1S	2.49(1)	9(1)					
1Br	2.43(1)	5(1)	3(1)	0.0354	679.014	53.057	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	4(1)	0.0331	634.339	49.566	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	5(1)	4(1)	0.0324	622.026	48.604	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	5(1)	4(1)	0.0333	638.954	49.927	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.06(1)	0(1)					
1S	2.48(1)	9(1)					
1Br	2.43(1)	5(1)	3(1)	0.0379	727.390	56.837	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	3(1)	0.0350	671.280	52.453	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	0(1)					
1S	2.49(1)	9(1)					
1Br	2.44(1)	5(1)	4(1)	0.0337	645.779	50.460	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
4N/O	2.07(1)	1(1)					
1S	2.50(1)	9(1)					
1Br	2.45(1)	5(1)	4(1)	0.0341	655.040	51.184	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.49(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0357	770.818	60.230	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	5(1)	0.0341	653.844	51.090	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	3(1)					
1S	2.50(1)	7(1)					
1Br	2.46(1)	4(1)	5(1)	0.0341	654.930	51.175	5

Ni-N(2.0) Ni-S(2.2) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.06(3)	5(2)					
1S	2.29(3)	3(3)					
1Br	3.30(0.11)	13(13)	0(3)	0.1361	2610.773	204.001	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.49(1)	8(1)					
1Br	2.44(1)	4(1)	4(1)	0.0367	704.055	55.014	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0332	637.557	49.818	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.08(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0320	613.907	47.970	5

Ni-N(2.0) Ni-S(2.3) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.05(2)	5(1)					
1S	2.29(2)	3(2)					
1Br	2.75(3)	8(3)	neg1(3)	0.1023	1962.502	153.346	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.49(1)	8(1)					
1Br	2.44(1)	4(1)	3(1)	0.0387	742.083	57.985	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.44(1)	4(1)	4(1)	0.0340	653.134	51.035	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0317	608.698	47.563	5

Ni-N(2.0) Ni-S(2.4) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(1)	4(1)					
1S	2.64(2)	3(2)					
1Br	3.38(8)	12(9)	7(1)	0.0803	1540.754	120.392	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.49(1)	8(1)					
1Br	2.43(1)	4(1)	3(1)	0.0405	776.627	60.684	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.49(1)	8(1)					
1Br	2.44(1)	4(1)	3(1)	0.0352	676.183	52.836	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0323	619.319	48.392	5

Ni-N(2.0) Ni-S(2.5) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.11(1)	4(1)					
1S	2.64(2)	3(2)					
1Br	3.38(8)	12(9)	7(1)	0.0785	1506.073	117.682	5

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.49(2)	8(1)					
1Br	2.43(1)	4(1)	3(1)	0.0434	832.134	65.021	5

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.4)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.49(1)	8(1)					
1Br	2.44(1)	4(1)	3(1)	0.0377	723.377	56.523	5

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.44(1)	4(1)	3(1)	0.0342	656.791	51.320	5

Ni-N(2.0) Ni-S(2.6) Ni-Br(2.6)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.07(1)	2(1)					
1S	2.50(1)	8(1)					
1Br	2.45(1)	4(1)	4(1)	0.0329	631.170	49.318	5

Table K.5. Additional Fits for Zn(II) WT-PHD2 in Buffer with 50 mM PBS, 150 mM NaBr at pH 7.2.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.19(2)	0.4(1.7)	11.3(5.4)	0.3044	3908.129	476.420	3
3N/O	2.18(2)	2.1(1.4)	9.9(3.4)	0.1989	2553.748	311.314	3
4N/O	2.18(2)	3.5(1.2)	8.7(2.5)	0.1504	1930.587	235.348	3
5N/O	2.17(2)	4.9(1.3)	7.6(2.2)	0.1399	1796.001	218.941	3
6N/O	2.17(2)	6.3(1.4)	6.5(2.3)	0.1537	1973.523	240.582	3
7N/O	2.16(2)	7.7(1.7)	5.4(2.4)	0.1828	2346.555	286.056	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.28(2)	3.7(1.0)	6.9(4.3)	0.1290	1655.849	201.856	3
3S	2.28(1)	5.9(0.7)	8.1(2.4)	0.0552	708.734	86.398	3
4S	2.28(1)	7.8(0.5)	9.1(1.7)	0.0334	429.294	52.333	3
5S	2.28(1)	9.5(0.6)	9.9(1.8)	0.0383	491.630	59.932	3
6S	2.27(1)	11.1(0.8)	10.7(2.1)	0.0570	731.646	89.191	3
7S	2.27(2)	12.7(1.0)	11.4(2.6)	0.0826	1060.931	129.333	3

Ni-N(2.0) Ni-N(2.2)

N	Radius Å	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.12(2)	1.6(1.7)					
1N/O	2.23(2)	4.6(1.4)	7.3(3.0)	0.1078	1383.420	223.020	5
2N/O	2.09(2)	0.6(1.6)					
2N/O	2.21(1)	2.1(1.2)	5.4(2.2)	0.0777	997.061	160.735	5
3N/O	2.12(2)	1.1(1.6)					
1N/O	2.23(2)	3.5(1.3)	5.9(2.3)	0.0774	993.760	160.203	5
4N/O	2.12(2)	3.5(1.7)					
1N/O	2.22(2)	2.7(1.3)	4.8(2.1)	0.0768	985.713	158.906	5
3N/O	2.09(2)	2.1(1.9)					
2N/O	2.21(2)	1.3(1.3)	4.3(2.1)	0.0796	1021.918	164.742	5
5N/O	2.12(2)	5.7(2.1)					
1N/O	2.21(2)	2.2(1.5)	3.(2.3)	0.0937	1203.040	193.941	5
4N/O	2.09(2)	4.7(2.5)					
2N/O	2.20(2)	0.5(1.5)	3.2(2.3)	0.0984	1262.911	203.593	5
3N/O	2.07(3)	3.2(2.6)					
3N/O	2.19(2)	0.5(1.5)	2.9(2.3)	0.1057	1356.452	218.672	5
6N/O	2.12(3)	7.8(2.6)					
1N/O	2.21(2)	1.8(1.7)	2.9(2.6)	0.1203	1544.988	249.066	5
5N/O	2.09(3)	7.4(3.3)					
2N/O	2.20(2)	0.1(1.8)	2.2(2.6)	0.1253	1608.707	259.338	5
4N/O	2.07(3)	6.5(3.9)					
3N/O	2.19(2)	1.3(1.9)	2.0(2.6)	0.1338	1717.797	276.925	5

Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.22(2)	3.7(1.3)					
1S	2.32(1)	0.4(1.1)	11.2(2.4)	0.0284	365.124	58.861	5

2S	2.19(1)	5.5(1.1)					
2S	2.30(1)	2.9(0.7)	12.(1.5)	0.0117	149.971	24.177	5
3S	2.28(1)	3.8(0.6)					
1S	2.15(1)	2.8(1.1)	12.2(1.5)	0.0131	168.733	27.201	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.29(1)	4.5(0.7)					
2S	2.17(2)	6.8(1.5)	13.8(1.5)	0.0133	170.614	27.505	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.29(1)	7.5(0.6)					
2S	2.54(7)	24.5(13.4)	6.8(2.3)	0.0252	323.403	52.135	5
3S	2.17(2)	11.9(3.0)					
3S	2.28(1)	5.5(1.0)	15.1(2.1)	0.0230	294.834	47.530	5
6S							
1S			No Fit	No Fit	No Fit	No Fit	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.27(1)	6.8(1.2)					
3S	2.15(3)	13.8(4.4)	15.5(2.4)	0.0309	397.308	64.050	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	1.7(1.3)					5
1S	2.33(1)	0.4(0.8)	0.4(2.8)	0.0413	530.518	85.524	
1N/O							5
2S			No Fit	No Fit	No Fit	No Fit	
2N/O	2.05(2)	4.5(1.1)					
2S	2.30(1)	3.6(0.4)	5.2(1.5)	0.0112	143.178	23.082	5
3N/O	2.10(1)	4.2(0.9)					
1S	2.33(1)	1.1(0.6)	0.3(1.7)	0.0162	207.349	33.427	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O			No Fit	No Fit	No Fit	No Fit	5

4S							
4N/O	2.11(1)	6.7(0.8)					
1S	2.33(1)	1.7(0.5)	0.7(1.3)	0.0098	125.437	20.222	5
2N/O	2.03(3)	8.7(2.7)					
3S	2.29(1)	6.0(0.6)	7.3(1.9)	0.0160	204.984	33.045	5
3N/O	2.07(2)	8.1(1.3)					
2S	2.31(1)	4.2(0.5)	4.1(1.5)	0.0096	123.276	19.873	5
5N/O	2.13(2)	9.2(1.0)					
1S	2.32(1)	2.0(0.6)	1.1(1.6)	0.0126	161.340	26.009	5
1N/O	2.45(1)	0(1.1)					
5S	2.27(1)	10.7(0.6)	12.4(1.8)	0.0150	192.457	31.026	5
4N/O	2.01(3)	11.6(1.8)					
2S	2.31(1)	4.7(0.6)	2.6(2.0)	0.0110	141.233	22.768	5
2N/O	2.10(0.15)	24.4(2.6)					
4S	2.28(1)	8.0(0.8)	8.0(3.3)	0.0272	348.844	56.237	5
3N/O	2.08(6)	15.3(4.8)					
3S	2.29(1)	6.5(0.7)	5.9(2.6)	0.0183	235.209	37.910	5
6N/O	2.14(2)	11.6(1.4)					
1S	2.32(1)	2.1(0.8)	1.5(2.1)	0.0200	256.880	41.411	5
1N/O	2.44(1)	0.5(1.1)					
6S	2.27(1)	12.5(0.7)	12.4(2.0)	0.0192	246.236	39.695	5
5N/O	2.14(3)	14.2(2.5)					
2S	2.31(1)	5.0(0.7)	0.9(2.5)	0.0118	246.236	24.399	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.12(6)	18.8(7.0)					
3S	2.30(1)	6.6(0.8)	4.56(3.2)	0.0182	233.229	37.599	5
3N/O	2.14(0.11)	28.8(29.2)					
4S	2.29(1)	8.0(0.8)	7.3(3.8)	0.0262	336.042	54.173	5

Table K.6. Additional Fits for Zn(II) WT-PHD2 in Buffer with 50 mM PBS, 150 mM NaBr at pH 7.2.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.19(1)	1(1)	11(1)	0.3237	4284.338	218.147	3
3N/O	2.18(1)	2(1)	10(1)	0.2196	2907.086	148.021	3
4N/O	2.18(1)	4(1)	9(2)	0.1720	2276.298	115.903	3
5N/O	2.17(1)	5(1)	8(2)	0.1614	2136.804	108.801	3
6N/O	2.17(1)	6(1)	7(2)	0.1749	2314.671	117.857	3
7N/O	2.16(1)	8(1)	5(2)	0.2033	2691.275	137.033	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.29(1)	4(1)	7(3)	0.1481	1960.900	99.844	3
3S	2.28(1)	6(1)	8(2)	0.0753	996.292	50.729	3
4S	2.28(1)	8(1)	9(1)	0.0538	712.226	36.265	3
5S	2.28(1)	10(1)	10(1)	0.0586	775.188	39.471	3
6S	2.27(1)	11(1)	11(2)	0.0769	1018.095	51.839	3
7S	2.27(1)	13()	11(2)	0.1021	1351.131	68.796	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.12(1)	2(1)					
1N/O	2.24(1)	5(1)	8(2)	0.1304	1726.061	97.851	5
2N/O	2.09(1)	1(1)					
2N/O	2.21(1)	2(1)	6(2)	0.1004	1329.105	75.348	5
3N/O	2.12(1)	1(1)					
1N/O	2.23(1)	3(1)	6(2)	0.1012	1339.661	75.946	5
4N/O	2.12(1)	4(1)					
1N/O	2.22(1)	3(1)	5(1)	0.1007	1332.417	75.535	5
3N/O	2.09(1)	2(1)					
2N/O	2.21(1)	1(1)	4(1)	0.1023	1354.413	76.782	5
5N/O	2.12(1)	6(1)					
1N/O	2.21(1)	2(1)	4(2)	0.1172	1551.033	87.929	5
4N/O	2.09(2)	5(2)					
2N/O	2.21(1)	1(1)	3(2)	0.1205	1594.945	90.418	5
3N/O	2.07(2)	3(2)					
3N/O	2.19(1)	1(1)	3(2)	0.1266	1676.138	95.021	5
6N/O	2.12(2)	8(2)					
1N/O	2.21(1)	2(1)	3(2)	0.1432	1895.601	107.463	5

5N/O	2.09(2)	8(2)					
2N/O	2.20(1)	1(1)	2(2)	0.1467	1941.827	110.083	5
4N/O	2.07(2)	7(3)					
3N/O	2.19(1)	1(1)	2(2)	0.1541	2040.117	115.655	5

Zn-S(2.2) Zn-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.22(1)	4(1)					
1S	2.33(1)	1(1)	11(2)	0.0477	631.890	35.822	5
2S	2.19(1)	6(1)					
2S	2.30(1)	3(1)	13(1)	0.0321	425.096	24.099	5
3S	2.29(1)	4(1)					
1S	2.15(1)	3(1)	12(1)	0.0338	447.107	25.347	5
4S	2.29(1)	8(1)					
1S	2.59(5)	13(6)	8(2)	0.0470	622.646	35.298	5
3S	2.29(1)	5(1)					
2S	2.17(1)	7(1)	14(1)	0.0341	451.267	25.583	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.29(1)	8(1)					
2S	2.55(5)	24(11)	7(2)	0.0454	601.197	34.082	5
3S	2.17(2)	12(3)					
3S	2.28(1)	6(1)	15(2)	0.0435	576.064	32.657	5
6S	2.29(1)	11(1)					
1S	2.59(1)	5(1)	9(1)	0.0323	427.347	24.227	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.27(1)	7(1)					
3S	2.15(2)	14(3)	15(2)	0.0517	684.227	38.789	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	2(1)					5
1S	2.33(1)	1(1)	1(2)	0.0618	817.877	46.366	
1N/O							5
2S			No Fit	No Fit	No Fit	No Fit	

2N/O 2S	2.06(2) 2.30(1)	5(1) 4(1)	5(2)	0.0322	425.815	24.140	5
3N/O 1S	2.11(1) 2.33(1)	4(1) 1(1)	1(2)	0.0375	496.307	28.136	5
1N/O 3S			No Fit	No Fit	No Fit	No Fit	5
1N/O 4S			No Fit	No Fit	No Fit	No Fit	5
4N/O 1S	2.11(1) 2.33(1)	7(1) 2(1)	1(1)	0.0316	418.930	23.749	5
2N/O 3S	2.03(3) 2.29(1)	9(2) 6(1)	7(2)	0.0308	407.148	23.081	5
3N/O 2S	2.07(2) 2.31(1)	8(1) 4(1)	4(2)	0.0367	485.294	27.512	5
5N/O 1S	2.12(2) 2.32(1)	9(1) 2(1)	1(2)	0.0348	460.395	26.100	5
1N/O 5S	2.45(1) 2.27(1)	1(1) 11(1)	13(2)	0.0343	453.624	25.716	5
4N/O 2S	2.10(3) 2.31(1)	12(2) 5(1)	3(2)	0.0477	631.061	35.775	5
2N/O 4S	2.10(0.12) 2.28(1)	25(19) 8(1)	8(3)	0.0324	428.806	24.309	5
3N/O 3S	2.08(5) 2.29(1)	15(4) 7(1)	6(2)	0.0392	518.346	29.385	5
6N/O 1S	2.13(2) 2.32(1)	12(1) 2(1)	1(2)	0.0424	561.727	31.845	5
1N/O 6S	2.44(1) 2.27(1)	1(1) 13(1)	13(2)	0.0387	511.841	29.017	5
5N/O 2S	2.13(3) 2.31(1)	14(3) 5(1)	1(3)	0.0335	443.831	25.161	5
2N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.12(5)	19(6)	5(3)	0.0467	617.856	35.027	5

3S	2.29(1)	7(1)					
3N/O	2.14(9)	29(24)					
4S	2.29(1)	8(1)	7(3)	0.0391	517.758	29.352	5

Zn-N(2.0) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(2)	1(1)					5
1Br	2.48(2)	7(2)	7(4)	0.2171	2874.184	162.939	
1N/O	1.95(4)	2(3)					5
2Br	2.34(2)	7(1)	neg30(7)	0.2412	3193.193	181.024	
2N/O	1.96(4)	5(3)					
2Br	2.34(2)	7(1)	neg28(7)	0.2202	2915.082	165.257	5
3N/O	2.16(1)	3(1)					
1Br	2.48(2)	7(2)	7(2)	0.1322	1750.179	99.218	5
1N/O	1.93(4)	3(3)					
3Br	2.33(2)	9(1)	neg31(5)	0.1849	2447.863	138.771	5
1N/O	2.42(4)	0(2)					
4Br	2.31(3)	11(1)	neg35(6)	0.1553	2055.409	116.522	5
4N/O	2.16(1)	4(1)					
1Br	2.47(1)	8(1)	6(2)	0.0922	1220.073	69.167	5
2N/O	1.93(4)	6(3)					
3Br	2.34(2)	9(1)	neg30(5)	0.1708	2261.084	128.182	5
3N/O	2.17(1)	3(1)					
2Br	2.49(2)	12(2)	7(2)	0.1349	1785.728	101.234	5
5N/O	2.17(1)	5(1)					
1Br	2.91(5)	12(5)	8(2)	0.1421	1880.697	106.618	5
1N/O	1.90(4)	4(3)					
5Br	2.33(2)	11(1)	neg33(4)	0.1327	1756.869	99.598	5
4N/O	2.16(1)	5(1)					
2Br	2.49(2)	12(2)	6(2)	0.0961	1271.644	72.090	5
2N/O	1.91(4)	8(3)					
4Br	2.33(2)	10(1)	neg32(5)	0.1419	1878.506	106.493	5
3N/O	2.17(1)	3(1)					
3Br	2.50(2)	15(2)	7(2)	0.1383	1831.176	103.810	5

6N/O	2.17(1)	6(1)					
1Br	2.90(5)	12(6)	6(2)	0.1543	2042.119	115.769	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.16(1)	6(1)					
2Br	2.48(1)	12(2)	5(1)	0.0850	1124.904	63.771	5
2N/O	1.89(4)	9(4)					
5Br	2.33(2)	11(1)	neg33(4)	0.1236	1635.880	92.739	5
4N/O	2.17(1)	5(1)					
3Br	2.49(2)	16(2)	6(2)	0.1004	1329.462	75.368	5
3N/O	1.90(4)	11(4)					
4Br	2.33(2)	10(1)	neg32(5)	0.1354	1792.523	101.619	5

Zn-N(2.0) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.17(1)	3(1)					
1Imd	2.02(2)	1(2)	4(2)	0.1460	1932.602	109.560	5
4N/O	2.15(1)	3(1)					
1Imd	2.21(3)	0(2)					
1Imd	2.03(2)	1(2)	4(1)	0.1114	1475.133	94.320	7
3N/O	2.15(2)	2(1)					
1Imd	1.98(3)	1(5)					
1Imd	2.10(4)	3(5)					
1Imd	2.22(3)	3(3)	3(2)	0.1139	1508.068	110.565	9
2N/O	2.16(2)	0(2)					
1Imd	2.24(3)	3(6)					
1Imd	1.66(7)	17(14)					
1Imd	2.02(9)	1(14)					
1Imd	2.12(6)	2(14)	6(3)	0.1127	1491.593	128.148	11
1N/O	2.15(3)	2(2)					
1Imd	2.06(3)	11(4)					
1Imd	2.27(3)	10(4)					
1Imd	2.16(3)	12(4)					
1Imd	1.96(4)	6(4)					
1Imd	1.69(0.22)	27(44)	4(3)	0.1578	2088.774	216.686	13
4N/O	2.17(1)	2(1)					
1Imd	2.03(2)	0(2)	5(2)	0.1461	1933.997	109.639	5
3N/O	2.16(1)	2(1)	5(1)	0.1100	1455.934	93.092	7

1Imd	2.04(2)	0(2)					
1Imd	2.21(2)	1(2)					
2N/O	2.16(2)	1(2)					
1Imd	2.23(3)	5(3)					
1Imd	2.11(3)	5(4)					
1Imd	2.00(3)	3(4)	4(2)	0.1279	1693.634	124.170	9
1N/O	2.14(3)	2(2)					
1Imd	2.05(3)	11(3)					
1Imd	2.27(3)	10(3)					
1Imd	2.16(3)	12(3)					
1Imd	1.95(3)	7(3)	3(2)	0.1655	2190.071	188.156	11
0N/O							
1Imd	2.27(3)	13(5)					
1Imd	1.98(3)	14(8)					
1Imd	2.08(3)	17(7)					
1Imd	1.90(5)	6(11)					
1Imd	2.18(3)	16(6)	0(3)	0.2835	3752.545	322.393	11
3N/O	2.18(2)	3(1)					
1Imd	2.13(8)	7(9)	8(2)	0.1814	2401.459	136.140	5
2N/O	2.17(1)	0(1)					
1Imd	2.06(2)	1(2)					
1Imd	2.21(2)	2(1)	6(2)	0.1375	1819.815	116.359	7
1N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
1Imd	2.15(3)	13(3)					
1Imd	1.96(4)	7(4)					
1Imd	2.05(3)	12(3)					
1Imd	2.26(2)	11(3)	2(2)	0.2875	3805.863	279.029	9
2N/O	2.19(2)	1(2)					
1Imd	2.16(8)	5(8)	9(3)	0.2428	3214.078	182.208	5
1N/O							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7
0N/O							
1Imd	2.12(2)	9(2)					
1Imd	2.02(3)	6(2)					
1Imd	2.24(2)	8(2)	4(3)	0.3176	4204.623	268.844	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.13(2)	1(1)					
1S	2.34(1)	1(1)					
1Br	1.96(3)	12(2)	1(2)	0.0451	597.451	38.201	7
1N/O	2.02(2)	2(1)					
2S	2.29(1)	4(1)					
1Br	2.44(4)	13(5)	neg8(3)	0.0426	563.830	36.051	7
1N/O	2.03(3)	0(1)					
1S	2.28(2)	1(1)					
2Br	2.46(4)	13(3)	neg8(4)	0.0922	1219.876	77.999	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	2(1)					
1S	2.31(1)	1(1)					
1Br	2.49(4)	13(4)	neg3(3)	0.0524	693.240	44.326	7
1N/O	1.37(0.12)	18(19)					
2S	2.25(3)	5(1)					
1Br	2.43(3)	7(2)	neg13(5)	0.1007	1333.417	85.259	7
1N/O	2.04(3)	0(1)					
1S	2.29(2)	1(1)					
2Br	2.47(4)	14(3)	neg7(4)	0.0965	1277.726	81.698	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	3(1)					
1S	2.30(2)	1(1)					
1Br	2.48(4)	12(4)	neg5(3)	0.0549	726.482	46.451	7
1N/O	2.01(2)	2(1)					
2S	2.28(1)	4(1)					
1Br	2.43(4)	13(5)	neg10(3)	0.0416	550.025	35.169	7
1N/O	2.02(3)	0(2)					
1S	2.27(2)	1(1)					
2Br	2.45(4)	12(3)	neg10(4)	0.0909	1203.709	76.965	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	3(1)					
1S	2.31(2)	1(1)	neg4(3)	0.0557	737.887	47.181	7

1Br	2.48(4)	13(4)					
1N/O	2.02(2)	2(1)					
2S	2.29(1)	4(1)					
1Br	2.43(4)	14(6)	neg9(2)	0.0420	556.552	35.586	7
1N/O	2.03(3)	0(2)					
1S	2.28(2)	1(1)					
2Br	2.46(4)	13(3)	neg9(4)	0.0960	1270.816	81.256	7

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.06(2)	3(1)					
1S	2.30(2)	1(1)					
1Br	2.47(3)	11(4)	neg6(3)	0.0558	738.086	47.193	7
1N/O	2.01(2)	2(1)					
2S	2.28(2)	4(1)					
1Br	2.42(3)	13(5)	neg11(2)	0.0397	525.045	33.571	7
1N/O	1.89(4)	3(3)					
1S	2.55(3)	1(2)					
2Br	2.28(3)	7(1)	neg41(7)	0.1509	1997.102	127.695	7

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	3(1)					
1S	2.31(2)	1(1)					
1Br	2.48(4)	12(4)	neg5(3)	0.0568	752.016	48.084	7
1N/O	2.01(2)	2(1)					
2S	2.28(1)	4(1)					
1Br	2.42(4)	14(5)	neg10(2)	0.0401	531.365	33.976	7
1N/O	2.02(3)	0(2)					
1S	2.28(2)	1(1)					
2Br	2.45(4)	13(3)	neg10(4)	0.0938	1241.452	79.378	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.13(2)	4(2)					
1S	2.34(1)	2(1)					
1Br	1.97(4)	16(5)	2(2)	0.0335	443.506	28.358	7
2N/O	2.06(2)	5(1)					
2S	2.31(1)	4(1)					
1Br	2.40(5)	17(8)	neg5(2)	0.0290	383.922	24.548	7

1N/O	2.02(2)	3(2)					
3S	2.30(1)	6(1)					
1Br	2.37(4)	13(5)	neg8(2)	0.0267	353.828	22.624	7
2N/O	2.23(1)	1(1)					
1S	1.80(2)	15(3)					
2Br	2.08(1)	11(1)	10(1)	0.0395	522.933	33.436	7
1N/O	2.06(3)	4(2)					
1S	2.05(3)	1(2)					
3Br	2.33(2)	7(1)	neg35(6)	0.1233	1631.662	104.329	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	5(1)					
1S	2.32(1)	2(1)					
1Br	2.47(5)	16(6)	neg2(2)	0.0354	468.465	29.954	7
2N/O	2.05(2)	5(2)					
2S	2.30(1)	4(1)					
1Br	2.39(5)	16(7)	neg7(2)	0.0299	395.783	25.306	7
1N/O	2.01(2)	4(2)					
3S	2.30(1)	7(1)					
1Br	2.36(3)	11(4)	neg9(2)	0.0263	348.137	22.260	7
2N/O	2.08(2)	3(1)					
1S	2.31(1)	1(1)					
2Br	2.48(4)	19(5)	neg4(3)	0.0574	760.035	48.597	7
1N/O	2.03(3)	1(2)					
1S	2.28(2)	1(1)					
3Br	2.45(4)	16(3)	neg10(5)	0.0940	1244.752	79.590	7

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(2)	5(1)					
1S	2.32(1)	2(1)					
1Br	2.46(5)	16(7)	neg2(2)	0.0371	491.020	31.396	7
2N/O	2.05(2)	6(2)					
2S	2.30(1)	4(1)					
1Br	2.39(4)	15(7)	neg8(2)	0.0297	393.671	25.171	7
1N/O	1.38(4)	13(5)					
3S	2.29(1)	6(1)	neg11(2)	0.0368	487.317	31.159	7

1Br	1.94(2)	14(2)					
2N/O	2.07(2)	3(1)					
1S	2.31(2)	1(1)					
2Br	2.47(4)	18(5)	neg5(3)	0.0585	774.406	49.516	7
1N/O	1.87(5)	4(4)					
1S	2.55(3)	2(2)					
3Br	2.28(3)	10(1)	neg42(6)	0.1302	1722.847	110.159	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	5(1)					
1S	2.32(1)	1(1)					
1Br	2.48(4)	17(6)	neg1(2)	0.0323	427.845	27.356	7
2N/O	2.06(2)	5(1)					
2S	2.31(1)	4(1)					
1Br	2.40(5)	18(8)	neg5(2)	0.0285	377.320	24.126	7
1N/O	2.02(2)	3(2)					
3S	2.30(1)	6(1)					
1Br	2.37(4)	14(5)	neg8(2)	0.0262	346.627	22.163	7
2N/O	2.09(2)	2(1)					
1S	2.32(1)	1(1)					
2Br	2.49(5)	21(6)	neg2(3)	0.0546	722.145	46.174	7
1N/O	2.05(3)	0(2)					
1S	2.29(2)	1(1)					
3Br	2.48(5)	19(4)	neg6(4)	0.0999	1322.614	84.568	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	5(1)					
1S	2.32(1)	2(1)					
1Br	2.47(5)	17(7)	neg1(2)	0.0352	465.556	29.768	7
2N/O	2.05(2)	5(2)					
2S	2.31(1)	4(1)					
1Br	2.39(5)	17(7)	neg7(2)	0.0294	389.035	24.875	7
1N/O	2.01(2)	4(2)					
3S	2.30(1)	6(1)					
1Br	2.37(3)	12(4)	neg9(2)	0.0258	341.232	21.818	7
2N/O	2.08(2)	3(1)	neg3(3)	0.0581	769.467	49.200	7

1S	2.32(1)	1(1)					
2Br	2.48(5)	20(6)					
1N/O	2.04(3)	1(2)					
1S	2.29(2)	1(1)					
3Br	2.46(4)	18(4)	neg8(5)	0.0997	1320.242	84.416	7

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	5(1)					
1S	2.32(1)	2(1)					
1Br	2.47(5)	18(7)	neg2(2)	0.0368	487.767	31.188	7
2N/O	2.05(2)	6(2)					
2S	2.30(1)	4(1)					
1Br	2.39(4)	16(7)	neg8(2)	0.0293	387.368	24.768	7
1N/O	2.01(2)	4(2)					
3S	2.30(1)	7(1)					
1Br	2.37(3)	11(4)	neg10(2)	0.0250	330.811	21.152	7
2N/O	2.08(2)	3(1)					
1S	2.31(1)	1(1)					
2Br	2.48(5)	20(6)	neg4(3)	0.0595	787.205	50.334	7
1N/O	2.03(3)	1(2)					
1S	2.28(2)	1(1)					
3Br	2.46(4)	17(4)	neg9(5)	0.0977	1293.309	82.694	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	0(1)					
1S	2.33(1)	0(0)					
1Imd	2.00(2)	3(1)	neg2(1)	0.0232	307.281	19.648	7
1N/O	2.10(1)	2(1)					
1S	2.33(1)	0(1)					
1Imd	1.99(2)	1(1)					
1Imd	2.14(3)	2(2)	neg2(1)	0.0246	325.093	23.834	9
0N/O							
1S	2.31(1)	1(1)					
1Imd	2.10(3)	6(2)					
1Imd	1.99(3)	3(2)					
1Imd	2.22(3)	4(2)	neg1(2)	0.0874	1157.099	84.833	9
1N/O	2.07(1)	0(1)	neg6(1)	0.0153	636.973	12.966	7

2S	2.30(1)	3(0)					
1Imd	1.98(1)	3(1)					
0N/O							
2S	2.30(1)	4(1)					
1Imd	2.11(9)	6(14)					
1Imd	2.01(7)	4(6)	neg5(2)	0.0474	202.787	40.089	7

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	0(1)					
1S	2.33(1)	0(0)					
1Imd	1.99(2)	3(1)	neg2(1)	0.0232	306.973	19.628	7
1N/O	2.10(1)	2(1)					
1S	2.33(1)	0(1)					
1Imd	1.99(2)	1(1)					
1Imd	2.14(3)	2(2)	neg2(1)	0.0251	332.198	24.355	9
0N/O							
1S	2.31(1)	1(1)					
1Imd	2.22(3)	4(2)					
1Imd	1.99(3)	3(2)					
1Imd	2.10(3)	6(2)	neg1(2)	0.0885	1170.919	85.847	9
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Imd	1.97(2)	3(1)	neg7(1)	0.0160	211.531	13.525	7
0N/O							
2S	2.30(1)	4(1)					
1Imd	2.01(0.12)	4(8)					
1Imd	2.09(0.15)	6(20)	neg6(2)	0.0486	643.564	41.150	7

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	0(1)					
1S	2.33(1)	1(0)					
1Imd	1.99(2)	3(1)	neg3(1)	0.0234	309.774	19.807	7
1N/O	2.10(1)	2(1)					
1S	2.33(1)	0(1)					
1Imd	2.13(3)	2(2)					
1Imd	1.99(2)	1(1)	neg2(2)	0.0258	341.208	25.016	9
0N/O							
1S	2.31(1)	1(1)	neg1(2)	0.0894	1183.614	86.777	9

1Imd	2.10(2)	6(2)					
1Imd	1.98(3)	3(2)					
1Imd	2.22(3)	4(2)					
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Imd	1.97(2)	3(1)	neg7(1)	0.0167	220.717	14.113	7
0N/O							
2S	2.30(1)	4(1)					
1Imd	2.03(0.16)	11(15)					
1Imd	2.03(6)	5(6)	neg7(2)	0.0496	655.992	41.944	7

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	0(1)					
1S	2.33(1)	0(0)					
1Imd	1.99(2)	3(1)	neg3(1)	0.0238	315.463	20.171	7
1N/O	2.10(1)	2(1)					
1S	2.33(1)	0(1)					
1Imd	1.98(2)	1(1)					
1Imd	2.13(3)	2(2)	neg3(2)	0.0267	353.909	25.947	9
0N/O							
1S	2.31(1)	1(1)					
1Imd	2.22(3)	4(2)					
1Imd	2.10(3)	6(2)					
1Imd	1.98(3)	3(2)	neg2(1)	0.0914	1209.595	88.682	9
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Imd	1.96(2)	3(1)	neg8(1)	0.0173	229.184	14.654	7
0N/O							
2S	2.30(1)	4(1)					
1Imd	2.03(5)	4(4)					
1Imd	2.02(0.15)	12(15)	neg7(2)	0.0509	673.704	43.077	7

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.18(2)	1(2)					
1S	2.81(9)	13(13)					
1Imd	2.17(9)	5(8)	9(3)	0.2456	3251.272	207.887	7
1N/O							
1S			No Fit	No Fit	No Fit	No Fit	9

1Imd							
1Imd							
0N/O							
1S	2.74(7)	8(8)					
1Imd	2.13(3)	9(2)					
1Imd	2.02(3)	6(3)					
1Imd	2.24(2)	8(2)	4(3)	0.3305	4374.156	320.694	9
1N/O	2.15(4)	1(3)					
2S	3.19(5)	7(5)					
1Imd	2.23(3)	1(2)	11(4)	0.3435	4546.984	438.819	7
0N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	7

Zn-N(2.0) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(2)	2(2)					
1Br	2.47(2)	7(2)					
1Imd	2.13(8)	6(7)	6(3)	0.1468	1942.795	124.222	7
1N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
1Br	2.46(3)	7(3)					
1Imd	2.22(3)	6(3)					
1Imd	2.11(3)	7(3)					
1Imd	2.00(3)	5(3)	1(3)	0.2222	2941.640	215.668	9
1N/O	1.97(5)	0(3)					
2Br	2.33(3)	6(1)					
1Imd	1.86(7)	4(5)	neg32(7)	0.2045	2706.984	173.085	7
0N/O							
2Br	2.46(2)	10(2)					
1Imd	2.17(3)	3(2)					
1Imd	2.05(3)	2(2)	0(4)	0.2697	3570.116	228.273	7

Zn-N(2.0) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(2)	2(2)	6(3)	0.1507	1994.775	127.546	7

1Br	2.48(2)	7(2)					
1Imd	2.13(8)	6(7)					
1N/O	2.15(2)	2(1)					
1Br	2.48(2)	7(2)					
1Imd	2.19(2)	2(1)					
1Imd	2.04(2)	2(2)	3(2)	0.1230	1628.113	119.366	9
0N/O							
1Br	2.46(3)	7(3)					
1Imd	2.11(3)	7(3)					
1Imd	2.01(3)	5(3)					
1Imd	2.22(3)	6(3)	1(3)	0.2254	2984.261	218.793	9
1N/O	1.97(5)	0(3)					
2Br	2.33(3)	7(1)					
1Imd	1.85(7)	4(5)	neg33(7)	0.2054	2718.696	173.834	7
0N/O							
2Br	2.32(3)	6(1)					
1Imd	1.82(7)	3(6)					
1Imd	1.96(5)	0(4)	neg3(7)	0.2193	2902.328	185.575	7

Zn-N(2.0) Zn-Br(2.5) Zn-Imd

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.17(2)	2(2)					
1Br	2.48(2)	7(2)					
1Imd	2.14(8)	6(7)	6(3)	0.1541	2039.849	130.428	7
1N/O	2.15(2)	2(1)					
1Br	2.48(2)	7(2)					
1Imd	2.04(2)	2(2)					
1Imd	2.19(2)	3(1)	3(2)	0.1252	1657.249	121.502	9
0N/O							
1Br	2.46(3)	8(3)					
1Imd	2.22(3)	7(3)					
1Imd	2.11(3)	8(3)					
1Imd	2.01(3)	5(3)	1(3)	0.2279	3017.088	221.200	9
1N/O	2.17(3)	0(3)					
2Br	2.49(3)	11(2)					
1Imd	2.14(8)	4(7)	5(4)	0.2571	3403.558	217.624	7
0N/O							
2Br	2.47(3)	10(2)					
1Imd	2.18(3)	3(2)					
1Imd	2.05(3)	2(2)	1(4)	0.2806	3713.844	237.463	7

Zn-N(2.0) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.17(2)	2(2)					
1Br	2.48(2)	8(2)					
1Imd	2.14(8)	6(8)	6(3)	0.1569	2077.002	132.804	7
1N/O							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O							
1Br	2.46(3)	8(3)					
1Imd	2.22(3)	7(3)					
1Imd	2.11(3)	8(3)					
1Imd	2.01(3)	5(3)	2(3)	0.2300	3045.139	223.256	9
1N/O	2.17(3)	0(3)					
2Br	2.49(3)	12(3)					
1Imd	2.14(7)	4(7)	6(4)	0.2609	3453.870	220.841	7
0N/O							
2Br	2.48(3)	11(2)					
1Imd	2.06(3)	2(2)					
1Imd	2.18(3)	4(2)	1(4)	0.2845	3765.661	240.777	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(1)	3(1)					
1S	2.33(1)	1(1)					
1Imd	2.00(2)	4(2)	neg1(1)	0.0191	252.523	16.146	7
2N/O	2.09(2)	4(1)					
2S	2.31(1)	4(0)					
1Imd	1.98(2)	5(2)	neg5(1)	0.0144	190.486	12.180	7
2N/O	2.11(1)	1(1)					
1S	2.33(1)	1(1)					
1Imd	2.17(3)	6(3)					
1Imd	1.99(2)	2(1)	neg1(1)	0.0119	157.508	11.548	9
1N/O	2.08(1)	0(1)					
2S	2.31(1)	4(0)					
1Imd	1.97(2)	3(1)					
1Imd	2.15(4)	9(5)	neg5(1)	0.0128	169.059	12.395	9
1N/O	2.09(1)	2(1)					
1S	2.32(1)	0(0)	0(1)	0.0125	165.750	14.240	11

1Imd	2.26(2)	2(1)					
1Imd	2.12(2)	4(1)					
1Imd	1.98(1)	2(1)					
0N/O							
2S	2.30(1)	4(1)					
1Imd	2.08(4)	2(4)					
1Imd	1.97(3)	1(4)					
1Imd	2.21(4)	0(4)	neg4(2)	0.0406	536.818	39.357	9

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(1)	3(1)					
1S	2.33(1)	1(1)					
1Imd	2.00(2)	4(2)	neg2(1)	0.0182	240.680	15.389	7
2N/O	2.09(2)	4(1)					
2S	2.31(1)	4(0)					
1Imd	1.97(2)	5(2)	neg6(1)	0.0147	194.903	12.462	7
2N/O	2.11(1)	1(1)					
1S	2.33(1)	1(1)					
1Imd	1.99(1)	2(1)					
1Imd	2.16(3)	5(3)	neg1(1)	0.0115	152.303	11.166	9
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Imd	1.97(0.18)	30(27)					
1Imd	1.97(2)	4(2)	neg7(2)	0.0143	189.937	13.925	9
1N/O	2.09(1)	2(1)					
1S	2.32(1)	0(1)					
1Imd	1.98(1)	2(1)					
1Imd	2.26(2)	2(2)					
1Imd	2.12(2)	4(1)	0(1)	0.0135	178.083	15.300	11
0N/O							
2S	2.30(1)	4(1)					
1Imd	2.06(5)	0(5)					
1Imd	2.19(5)	1(5)					
1Imd	1.96(4)	2(6)	neg5(2)	0.0429	567.203	41.585	9

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(1)	3(1)					
1S	2.33(1)	1(1)					
1Imd	1.99(2)	4(2)	neg2(1)	0.0178	235.485	15.057	7

2N/O	2.08(2)	4(1)					
2S	2.31(1)	4(0)					
1Imd	1.97(2)	5(2)	neg6(1)	0.0154	203.247	12.996	7
2N/O	2.11(1)	1(1)					
1S	2.33(1)	1(1)					
1Imd	1.99(1)	2(1)					
1Imd	2.16(3)	5(3)	neg1(1)	0.0116	153.017	11.219	9
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Imd	1.97(2)	4(2)					
1Imd	1.94(0.14)	29(26)	neg8(1)	0.0149	197.790	14.501	9
1N/O	2.09(1)	2(1)					
1S	2.33(1)	0(1)					
1Imd	2.12(2)	4(1)					
1Imd	1.98(1)	2(1)					
1Imd	2.26(2)	2(2)	neg1(1)	0.0143	189.011	16.239	11
0N/O							
2S	2.30(1)	4(1)					
1Imd	2.04(5)	1(5)					
1Imd	2.17(7)	3(7)					
1Imd	1.95(8)	6(12)	neg6(2)	0.0443	586.425	42.994	9

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.11(1)	3(1)					
1S	2.33(1)	1(1)					
1Imd	1.99(2)	4(2)	neg2(1)	0.0177	234.770	15.011	7
2N/O	2.08(2)	4(1)					
2S	2.30(1)	4(0)					
1Imd	1.97(2)	5(2)	neg6(1)	0.016	211.335	13.513	7
2N/O	2.11(1)	1(1)					
1S	2.33(1)	1(1)					
1Imd	2.16(3)	5(3)					
1Imd	1.98(1)	2(1)	neg1(1)	0.0119	157.005	11.511	9
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Imd	1.97(2)	4(2)					
1Imd	1.92(0.11)	27(24)	neg8(1)	0.0155	204.786	15.014	9
1N/O	2.09(1)	2(1)					
1S	2.33(1)	0(1)	neg1(1)	0.0151	200.205	17.200	11

1Imd	1.98(1)	2(1)					
1Imd	2.11(2)	4(1)					
1Imd	2.26(2)	2(2)					
0N/O							
2S	2.29(1)	4(1)					
1Imd	2.03(5)	1(5)					
1Imd	2.16(7)	3(8)					
1Imd	1.94(8)	7(12)	neg7(2)	0.0459	607.307	44.525	9

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.18(1)	1(1)					
1S	3.01(0.19)	23(34)					
1Imd	2.06(2)	0(2)	7(2)	0.1691	2238.505	143.130	7
2N/O	2.19(2)	1(2)					
2S	3.12(0.21)	34(43)					
1Imd	2.15(8)	5(8)	9(3)	0.233	3083.998	197.191	7
2N/O	2.17(2)	0(2)					
1S	3.12(7)	8(9)					
1Imd	2.06(3)	1(2)					
1Imd	2.21(3)	2(1)	6(2)	0.121	1601.623	117.424	9
1N/O	2.17(2)	2(2)					
2S	3.12(6)	11(7)					
1Imd	2.08(3)	3(2)					
1Imd	2.22(3)	3(1)	7(3)	0.1861	2463.948	180.646	9
1N/O							
1S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11

Zn-N(2.0) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.16(2)	4(2)					
1Br	2.47(2)	7(1)					
1Imd	2.13(8)	8(9)	5(2)	0.097	1284.429	82.126	7
2N/O	2.17(2)	2(2)					
2Br	2.49(2)	12(2)					
1Imd	2.15(8)	6(8)	6(3)	0.1519	2010.670	128.562	7
2N/O			No Fit	No Fit	No Fit	No Fit	9

1Br							
1Imd							
1Imd							
1N/O	1.97(5)	1(4)					
2Br	2.32(3)	6(1)					
1Imd	1.93(0.10)	4(12)					
1Imd	1.80(8)	3(8)	neg33(8)	0.1898	2512.564	184.210	9
1N/O	2.15(2)	2(2)					
1Br	2.47(2)	7(2)					
1Imd	2.23(7)	1(12)					
1Imd	2.13(7)	3(10)					
1Imd	2.02(4)	2(5)	3(2)	0.1037	1372.735	117.936	11
0N/O							
2Br	2.46(2)	11(3)					
1Imd	2.01(3)	4(3)					
1Imd	2.11(3)	7(3)					
1Imd	2.22(3)	6(3)	1(3)	0.2209	2924.085	214.381	9

Zn-N(2.0) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.16(2)	4(2)					
1Br	2.47(2)	8(2)					
1Imd	2.13(8)	8(9)	5(2)	0.1005	1330.912	85.099	7
2N/O	1.96(5)	3(3)					
2Br	2.33(3)	7(1)					
1Imd	1.82(8)	4(5)	neg32(8)	0.1968	2605.628	166.604	7
2N/O	2.15(1)	1(1)					
1Br	2.48(2)	8(2)					
1Imd	2.19(2)	1(1)					
1Imd	2.03(2)	1(1)	3(2)	0.0694	918.714	67.356	9
1N/O	2.15(2)	2(2)					
2Br	2.49(2)	12(2)					
1Imd	2.19(2)	2(1)					
1Imd	2.05(2)	2(2)	3(2)	0.1305	1727.645	126.663	9
1N/O	2.15(2)	2(2)					
1Br	2.47(2)	7(2)					
1Imd	2.23(7)	1(13)					
1Imd	2.13(7)	3(11)					
1Imd	2.02(4)	2(5)	3(2)	0.1065	1409.306	121.078	11
0N/O							
2Br	2.47(3)	11(3)	1(3)	0.2256	2986.019	218.922	9

1Imd	2.01(3)	4(3)					
1Imd	2.11(3)	7(3)					
1Imd	2.22(3)	6(3)					

Zn-N(2.0) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.16(2)	3(2)					
1Br	2.48(2)	8(2)					
1Imd	2.13(8)	8(9)	5(2)	0.1036	1371.856	87.717	7
2N/O	2.17(2)	2(2)					
2Br	2.49(2)	12(2)					
1Imd	2.16(8)	6(8)	6(3)	0.1601	2118.706	135.470	7
2N/O	2.15(1)	1(1)					
1Br	2.48(2)	8(2)					
1Imd	2.19(2)	1(1)					
1Imd	2.03(2)	1(1)	3(2)	0.0714	945.655	69.331	9
1N/O							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.15(2)	2(2)					
1Br	2.47(2)	8(3)					
1Imd	2.02(4)	2(5)					
1Imd	2.13(7)	3(11)					
1Imd	2.23(7)	2(12)	3(2)	0.1087	1439.004	123.629	11
0N/O							
2Br	2.47(3)	12(3)					
1Imd	2.11(3)	7(3)					
1Imd	2.01(3)	4(3)					
1Imd	2.23(3)	6(3)	1(3)	0.2292	3033.399	222.396	9

Zn-N(2.0) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.16(1)	1(1)					
1Br	2.47(2)	8(2)					
1Imd	2.03(2)	1(2)	3(2)	0.1064	1408.146	90.037	7
2N/O	2.13(2)	2(2)					
2Br	2.50(2)	13(2)					
1Imd	2.21(3)	0(2)	6(2)	0.157	2078.466	132.897	7
2N/O			No Fit	No Fit	No Fit	No Fit	9

1Br							
1Imd							
1Imd							
1N/O	2.15(2)	2(2)					
2Br	2.49(2)	12(2)					
1Imd	2.05(2)	2(2)					
1Imd	2.20(2)	2(1)	4(2)	0.1364	1805.548	132.375	9
1N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
2Br	2.47(3)	12(3)					
1Imd	2.23(3)	6(3)					
1Imd	2.01(3)	4(3)					
1Imd	2.12(3)	7(3)	1(3)	0.2322	3074.054	225.376	9

Zn-N(2.0) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.16(1)	1(1)					
1Br	2.47(2)	8(2)					
1Imd	2.03(2)	1(2)	3(2)	0.1064	1408.146	90.037	7
2N/O	2.13(2)	2(2)					
2Br	2.50(2)	13(2)					
1Imd	2.21(3)	0(2)	6(2)	0.157	2078.466	132.897	7

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.94(2)	5(2)	neg8(1)	0.0114	150.879	11.062	9
1S	2.23(1)	1(1)					
1S	2.35(1)	1(1)					
1Imd	2.11(5)	6(7)					
1Imd	1.98(2)	2(2)	neg7(2)	0.0318	421.435	30.898	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(1)	neg9(1)	0.0120	158.562	11.625	9

1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.94(2)	6(2)					
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	1.98(2)	2(2)					
1Imd	2.11(5)	6(8)	neg7(2)	0.0321	425.293	31.181	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.94(2)	6(2)	neg9(1)	0.0122	161.235	11.821	9
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	2.11(5)	7(9)					
1Imd	1.98(3)	3(2)	neg7(2)	0.0322	426.213	31.248	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.93(2)	6(2)	neg9(1)	0.0124	164.069	12.029	9
1S	2.22(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	1.99(2)	3(2)					
1Imd	1.97(0.20)	24(26)	neg9(2)	0.0318	420.783	30.850	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.94(2)	5(2)	neg9(1)	0.0125	165.762	12.153	9
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	2.11(5)	6(8)					
1Imd	1.98(3)	2(3)	neg7(2)	0.0339	449.222	32.935	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.94(2)	6(2)	neg9(1)	0.0127	167.644	12.291	9
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	1.99(0.20)	22(23)					
1Imd	1.99(2)	3(2)	neg9(2)	0.0340	450.068	32.997	9

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.93(2)	6(2)	neg9(1)	0.0129	171.281	12.558	9
1S	2.22(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	1.96(0.19)	24(27)					
1Imd	1.99(2)	3(2)	neg10(2)	0.0331	437.623	32.085	9

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	2(1)					
1Imd	1.93(2)	6(2)	neg10(1)	0.0129	171.029	12.539	9
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	1.99(2)	3(2)					
1Imd	1.97(0.19)	23(26)	neg10(2)	0.0348	460.406	33.755	9

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(2)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	1(1)					
1Imd	1.93(2)	6(2)	neg10(1)	0.0132	174.333	12.781	9
1S	2.22(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	1.94(0.18)	24(28)	neg10(2)	0.0337	446.478	32.734	9

1Imd	1.99(2)	3(2)					

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	0(1)					
1S	2.30(0.63)	3(28)					
1S	2.29(0.60)	3(15)					
1Imd	1.96(2)	3(2)	neg8(2)	0.0173	228.521	16.754	9
1S	2.22(1)	1(1)					
1S	2.34(1)	1(1)					
1Imd	1.94(0.17)	23(29)					
1Imd	1.99(2)	3(2)	neg10(2)	0.0351	464.019	34.020	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(2)	5(3)					
1S	2.25(2)	2(3)					
1S	2.34(1)	1(2)					
1Imd	1.97(2)	4(2)	neg6(1)	0.0130	171.731	12.591	9
1N/O	2.02(1)	1(1)					
1S	2.24(1)	2(1)					
1S	2.35(1)	2(1)					
1Imd	1.95(2)	4(2)					
1Imd	1.82(4)	18(8)	neg9(1)	0.0086	114.408	9.829	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	4(3)					
1S	2.35(1)	1(2)					
1S	2.25(2)	2(3)					
1Imd	1.97(2)	4(2)	neg6(1)	0.0135	179.057	13.128	9
1N/O	2.01(1)	1(1)					
1S	2.23(1)	2(1)					
1S	2.35(1)	2(1)					
1Imd	1.95(2)	4(2)					
1Imd	1.81(4)	16(7)	neg10(1)	0.0090	119.335	10.252	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	3(3)					
1S	2.32(5)	2(1)	neg6(1)	0.0139	184.403	13.520	9

1S	2.27(5)	6(11)					
1Imd	1.97(2)	4(2)					
1N/O	2.01(1)	1(1)					
1S	2.23(1)	2(1)					
1S	2.35(1)	2(1)					
1Imd	1.81(4)	15(6)					
1Imd	1.95(2)	4(2)	neg10(1)	0.0089	118.182	10.153	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	3(3)					
1S	2.32(4)	2(2)					
1S	2.27(5)	6(10)					
1Imd	1.97(2)	4(2)	neg6(1)	0.0141	186.174	13.649	9
1N/O	2.01(2)	1(1)					
1S	2.23(1)	2(1)					
1S	2.34(1)	2(1)					
1Imd	1.95(2)	4(2)					
1Imd	1.81(3)	14(5)	neg10(1)	0.0087	115.731	9.943	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	4(3)					
1S	2.34(1)	1(2)					
1S	2.25(2)	2(3)					
1Imd	1.97(2)	4(2)	neg6(1)	0.0137	181.617	13.315	9
1N/O	2.01(1)	1(1)					
1S	2.23(1)	2(1)					
1S	2.35(1)	2(1)					
1Imd	1.81(4)	15(7)					
1Imd	1.95(2)	5(2)	neg10(1)	0.0092	122.214	10.500	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	3(3)					
1S	2.33(6)	2(1)					
1S	2.27(7)	5(13)					
1Imd	1.97(2)	4(2)	neg6(2)	0.0142	188.037	13.786	9
1N/O	2.01(1)	1(1)					
1S	2.23(1)	2(1)					
1S	2.35(1)	2(1)					
1Imd	1.94(2)	4(2)	neg10(1)	0.0091	119.922	10.303	11

1Imd	1.81(4)	15(6)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	3(3)					
1S	2.32(5)	2(1)					
1S	2.27(6)	5(12)					
1Imd	1.97(2)	4(2)	neg6(2)	0.0144	190.035	13.933	9
1N/O	2.01(2)	1(1)					
1S	2.23(1)	2(1)					
1S	2.34(1)	2(1)					
1Imd	1.80(3)	13(5)					
1Imd	1.94(2)	4(2)	neg11(1)	0.0089	118.196	10.155	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	4(3)					
1S	2.34(3)	2(3)					
1S	2.25(4)	3(6)					
1Imd	1.97(2)	4(2)	neg6(2)	0.0146	192.635	14.123	9
1N/O	2.01(1)	1(1)					
1S	2.23(1)	2(1)					
1S	2.35(1)	2(1)					
1Imd	1.94(2)	4(2)					
1Imd	1.80(4)	15(6)	neg10(1)	0.0091	120.684	10.368	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	3(3)					
1S	2.33(7)	2(2)					
1S	2.26(7)	5(13)					
1Imd	1.96(2)	4(2)	neg7(2)	0.0147	195.014	14.298	9
1N/O	2.01(1)	1(1)					
1S	2.23(1)	2(1)					
1S	2.34(1)	2(1)					
1Imd	1.94(2)	4(2)					
1Imd	1.80(3)	13(5)	neg11(1)	0.0090	118.764	10.203	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.09(2)	4(3)	neg7(2)	0.0148	195.702	14.348	9

1S	2.25(3)	3(5)					
1S	2.34(2)	1(3)					
1Imd	1.96(2)	4(2)					
1N/O	2.01(2)	1(1)					
1S	2.23(1)	2(1)					
1S	2.34(1)	2(1)					
1Imd	1.80(3)	14(5)					
1Imd	1.94(2)	4(2)	neg11(1)	0.0094	124.477	10.694	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.11(1)	2(1)					
1S	2.33(1)	0(1)					
1Br	2.00(3)	12(3)					
1Imd	1.98(2)	3(2)	neg3(2)	0.0298	394.545	28.926	9
1S	2.29(2)	1(2)					
1Br	2.47(4)	9(3)					
1Imd	2.01(4)	1(4)					
1Imd	2.13(6)	2(6)	neg4(4)	0.0996	1317.845	96.619	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
1Br	2.49(5)	15(5)					
1Imd	2.00(3)	3(2)	neg4(2)	0.0463	613.471	44.977	9
1S	2.30(2)	2(1)					
1Br	2.47(4)	10(4)					
1Imd	2.02(4)	1(4)					
1Imd	2.14(6)	2(6)	neg4(3)	0.1020	1350.638	99.023	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	2(1)					
1S	2.31(1)	0(1)					
1Br	2.48(4)	14(5)					
1Imd	1.99(3)	2(2)	neg5(3)	0.0466	617.079	45.242	9
1S	2.29(2)	2(2)					
1Br	2.46(4)	10(4)					
1Imd	2.01(4)	2(5)					
1Imd	2.12(6)	2(7)	neg5(4)	0.1028	1360.906	99.776	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
1Br	2.48(5)	15(6)					
1Imd	1.99(3)	2(2)	neg5(2)	0.0481	636.907	46.695	9
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	2(1)					
1S	2.31(1)	0(1)					
1Br	2.47(5)	14(5)					
1Imd	1.99(3)	2(2)	neg6(3)	0.0468	619.791	45.440	9
1S	3.11(3)	1(2)					
1Br	2.48(3)	6(2)					
1Imd	2.18(2)	5(2)					
1Imd	2.07(3)	3(2)	3(3)	0.2168	2869.158	210.354	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
1Br	2.48(5)	15(6)					
1Imd	1.99(3)	2(2)	neg6(3)	0.0483	639.312	46.872	9
1S							
1Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.11(1)	1(1)					
1S	2.33(1)	1(1)					
1Br	2.02(5)	18(7)					
1Imd	1.98(2)	3(2)	neg2(1)	0.0189	250.121	18.338	9
1N/O	2.10(1)	2(1)					
1S	2.33(1)	1(1)					
1Br	2.45(7)	20(10)	neg2(2)	0.0249	329.975	28.349	11

1Imd	1.99(2)	1(1)					
1Imd	2.14(3)	3(3)					

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	1(1)					
1S	2.32(1)	1(1)					
1Br	2.48(7)	21(9)					
1Imd	1.99(2)	3(2)	neg2(2)	0.0226	299.201	21.936	9
1N/O	2.10(1)	2(1)					
1S	2.33(1)	1(1)					
1Br	2.45(8)	21(11)					
1Imd	2.15(3)	2(3)					
1Imd	1.99(2)	1(1)	neg2(2)	0.0252	333.250	28.631	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	1(1)					
1S	2.32(1)	1(1)					
1Br	2.47(8)	22(11)					
1Imd	1.99(2)	3(2)	neg3(2)	0.0230	304.586	22.331	9
1N/O	2.1(1)	2(1)					
1S	2.33(1)	1(1)					
1Br	2.44(9)	22(13)					
1Imd	1.99(2)	1(1)					
1Imd	2.14(3)	2(3)	neg2(2)	0.0267	353.595	30.379	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	1(1)					
1S	2.32(1)	1(1)					
1Br	2.48(0.10)	26(15)					
1Imd	1.99(2)	3(2)	neg3(2)	0.0233	308.780	22.638	9
1N/O	2.10(1)	2(1)					
1S	2.33(1)	1(1)					
1Br	2.43(0.10)	23(15)					
1Imd	1.99(2)	1(1)					
1Imd	2.14(3)	2(3)	neg2(2)	0.0267	353.097	30.336	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2N/O	2.10(1)	1(1)					
1S	2.32(1)	1(1)					
1Br	2.48(0.10)	25(15)					
1Imd	1.98(2)	3(2)	neg4(2)	0.0233	307.982	22.580	9
1N/O	2.16(2)	2(1)					
1S	3.06(6)	7(7)					
1Br	2.48(2)	7(2)					
1Imd	2.18(2)	3(1)					
1Imd	2.04(2)	3(1)	3(2)	0.0956	1265.104	108.689	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.10(1)	0(1)					
1S	2.33(1)	1(1)					
1Br	2.66(0.72)	50(127)					
1Imd	1.99(2)	3(1)	neg3(1)	0.0233	309.000	22.655	9
1N/O	2.10(2)	1(1)					
1S	2.33(1)	1(1)					
1Br	2.02(4)	13(4)					
1Imd	2.08(5)	7(6)					
1Imd	1.95(2)	2(2)	neg4(2)	0.0187	247.771	21.287	11

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(5)	15(6)					
1Imd	2.00(2)	2(1)	neg8(2)	0.0355	469.301	34.407	9

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	15(6)					
1Imd	2.00(2)	2(1)	neg8(2)	0.0353	466.897	34.231	9

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	15(5)					
1Imd	2.00(2)	2(1)	neg8(2)	0.0352	466.125	34.174	9

Zn-S(2.2) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(4)	15(6)					
1Imd	2.00(2)	2(1)	neg8(2)	0.0344	455.118	33.367	9

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	15(5)					
1Imd	2.00(2)	2(1)	neg8(2)	0.0342	452.901	33.205	9

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	15(5)					
1Imd	2.00(2)	2(1)	neg8(2)	0.0342	452.240	33.156	9

Zn-S(2.2) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(4)	15(6)					
1Imd	2.00(2)	2(1)	neg9(2)	0.0333	441.384	32.360	9

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(4)	15(5)					
1Imd	2.00(2)	2(1)	neg9(2)	0.0332	439.164	32.198	9

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	15(5)					
1Imd	2.00(2)	2(1)	neg9(2)	0.0331	438.447	32.145	9

Zn-S(2.2) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	0(1)					
1S	2.34(1)	0(1)					
1Br	1.99(2)	11(2)					
1Imd	1.94(2)	4(2)	neg10(1)	0.0193	254.920	18.690	9

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(4)	15(5)					
1Imd	1.99(2)	2(1)	neg9(2)	0.0320	423.260	31.032	9

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	15(5)					
1Imd	1.99(2)	2(1)	neg9(2)	0.0319	422.537	30.979	9

Zn-S(2.2) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	0(1)					
1S	2.34(1)	0(1)					
1Br	1.99(2)	11(2)					
1Imd	1.93(2)	4(2)	neg10(1)	0.0196	260.081	19.068	9

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	2.00(2)	2(1)	neg9(2)	0.0363	480.174	35.204	9

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(5)	16(6)					
1Imd	2.00(2)	2(1)	neg9(2)	0.0361	478.066	35.050	9

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(5)	16(6)					
1Imd	2.00(2)	2(1)	neg9(2)	0.0361	477.496	35.008	9

Zn-S(2.3) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	16(6)					
1Imd	2.00(2)	2(1)	neg9(2)	0.0361	477.507	35.009	9

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	1.99(2)	2(1)	neg9(2)	0.0351	464.162	34.030	9

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(4)	16(6)					
1Imd	1.99(2)	2(1)	neg9(2)	0.0349	462.049	33.875	9

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.77(4)	16(6)					
1Imd	1.99(2)	2(1)	neg9(2)	0.0349	461.422	33.829	9

Zn-S(2.3) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	1.99(2)	2(1)	neg9(2)	0.0337	445.689	32.676	9

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(4)	16(6)					
1Imd	1.99(2)	2(1)	neg9(2)	0.0336	445.053	32.629	9

Zn-S(2.3) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	0(1)					
1S	2.34(1)	0(1)					
1Br	1.99(2)	11(2)					
1Imd	1.93(2)	4(2)	neg10(1)	0.0203	268.748	19.703	9

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.34(1)	1(1)					
1S	2.23(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	2.00(2)	2(2)	neg9(2)	0.0389	514.547	37.724	9

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	1.99(2)	2(2)	neg9(2)	0.0359	474.629	34.798	9

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.34(1)	1(1)					
1S	2.23(1)	1(1)					
1Br	2.77(5)	15(6)					
1Imd	2.00(2)	2(2)	neg9(2)	0.0387	511.800	37.523	9

Zn-S(2.4) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.75(5)	16(6)					
1Imd	1.99(2)	2(1)	neg10(2)	0.0347	459.345	33.677	9

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.75(5)	16(6)					
1Imd	1.99(2)	2(1)	neg10(2)	0.0347	459.345	33.677	9

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	1.99(2)	2(1)	neg10(2)	0.0346	457.363	33.532	9

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	1.99(2)	2(1)	neg10(2)	0.0345	456.754	33.487	9

Zn-S(2.4) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.34(1)	1(1)					
1S	2.23(1)	1(1)					
1Br	2.76(5)	15(6)					
1Imd	1.99(2)	2(2)	neg10(2)	0.0377	499.420	36.615	9

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	1.99(2)	2(2)	neg10(2)	0.0358	474.375	34.779	9

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S	2.23(1)	1(1)					
1S	2.34(1)	1(1)					
1Br	2.76(5)	16(6)					
1Imd	1.99(2)	2(2)	neg10(2)	0.0358	473.719	34.731	9

Zn-S(2.5) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1S							
1S							
1Br							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	2(2)					
1S	2.35(2)	2(1)					
1S	2.24(2)	3(1)					
1Br	2.18(.11)	19(13)					
1Imd	1.95(2)	4(2)	neg8(2)	0.0094	123.850	10.640	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.02(2)	2(2)					
1S	2.35(2)	2(1)					
1S	2.24(2)	3(1)					
1Br	2.20(0.11)	19(12)					
1Imd	1.95(2)	4(2)	neg8(2)	0.0093	122.649	10.537	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	2(1)					
1S	2.26(2)	3(1)					
1S	2.37(2)	2(1)					
1Br	2.30(6)	14(6)					
1Imd	1.96(2)	4(2)	neg7(1)	0.0083	109.829	9.436	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	1.38(0.10)	16(15)					
1S	2.96(6)	8(7)					
1S	2.28(2)	0(1)					
1Br	2.47(3)	8(3)					
1Imd	2.02(3)	1(2)	neg8(4)	0.0878	1162.341	99.861	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

1N/O	2.05(2)	2(1)					
1S	2.26(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	10(4)					
1Imd	1.97(2)	4(1)	neg6(1)	0.0085	112.685	9.681	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.26(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	11(5)					
1Imd	1.97(2)	4(1)	neg6(1)	0.0084	111.257	9.558	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	2(1)					
1S	2.26(2)	3(1)					
1S	2.37(2)	2(1)					
1Br	2.32(5)	12(5)					
1Imd	1.97(2)	4(1)	neg6(1)	0.0083	109.570	9.414	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	1(2)					
1S	2.36(1)	1(1)					
1S	2.25(1)	2(1)					
1Br	2.75(5)	20(8)					
1Imd	1.97(2)	4(2)	neg7(2)	0.0110	145.955	12.540	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	9(4)					
1Imd	1.97(2)	4(1)	neg6(1)	0.0082	109.118	9.375	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.01(3)	2(2)					
1S	2.35(2)	2(1)					
1S	2.24(2)	3(1)	neg9(2)	0.0104	137.846	11.843	11

1Br	2.17(0.11)	18(14)
1Imd	1.94(3)	5(2)

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	11(4)					
1Imd	1.97(2)	4(1)	neg6(1)	0.0081	106.705	9.167	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.26(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	11(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0080	105.816	9.091	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	9(4)					
1Imd	1.97(2)	4(1)	neg6(1)	0.0081	107.083	9.200	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	9(4)					
1Imd	1.97(2)	4(1)	neg6(1)	0.0080	106.307	9.133	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	10(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0079	105.028	9.023	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	1(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	1(1)					
1Br	2.33(4)	11(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0079	104.256	8.957	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	10(4)					
1Imd	1.96(2)	4(1)	neg7(2)	0.0091	119.801	10.292	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.26(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	10(5)					
1Imd	1.97(2)	4(1)	neg7(2)	0.0089	117.963	10.135	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.26(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	11(5)					
1Imd	1.97(2)	4(1)	neg7(2)	0.0088	115.938	9.961	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	2(1)					
1S	2.26(2)	3(1)					
1S	2.37(2)	2(1)					
1Br	2.32(5)	12(5)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0087	114.704	9.855	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)	neg7(1)	0.0087	114.916	9.873	11

1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.33(5)	9(4)					
1Imd	1.97(2)	3(1)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	9(4)					
1Imd	1.97(2)	3(1)	neg7(1)	0.0086	113.683	9.767	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	10(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0085	112.035	9.625	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	11(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0084	111.069	9.542	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	2(1)					
1S	2.30(2)	0(1)					
1S	2.97(5)	7(4)					
1Br	2.48(3)	10(3)					
1Imd	1.98(3)	1(2)	neg6(3)	0.0319	422.520	36.300	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	9(4)	neg7(1)	0.0085	112.890	9.699	11

1Imd	1.97(2)	3(1)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	9(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0084	111.438	9.574	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	10(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0084	110.610	9.503	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	9(4)					
1Imd	1.96(2)	4(1)	neg7(2)	0.0092	121.675	10.454	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	10(4)					
1Imd	1.96(2)	4(1)	neg7(2)	0.0090	119.769	10.290	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.04(2)	2(1)					
1S	2.37(2)	2(1)					
1S	2.26(2)	3(1)					
1Br	2.31(5)	11(5)					
1Imd	1.96(2)	4(2)	neg7(2)	0.0099	130.903	11.246	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.32(5)	11(4)					
1Imd	1.96(2)	4(1)	neg7()	0.0088	116.245	9.987	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	2(1)					
1S	2.30(2)	0(1)					
1S	2.96(5)	7(4)					
1Br	2.48(3)	10(3)					
1Imd	1.98(3)	1(2)	neg7(3)	0.0327	432.498	37.157	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(5)	9(4)					
1Imd	1.96(2)	4(1)	neg7(2)	0.0090	119.237	10.244	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	10(4)					
1Imd	1.96(2)	4(1)	neg7(1)	0.0089	117.245	10.073	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	2(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	10(4)					
1Imd	1.97(2)	4(1)	neg7(1)	0.0088	116.066	9.972	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)	neg7(2)	0.0098	129.271	11.106	11

1S	2.38(2)	2(1)					
1S	2.27(2)	3(1)					
1Br	2.32(5)	9(4)					
1Imd	1.96(2)	4(2)					

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.33(5)	9(4)					
1Imd	1.96(2)	4(1)	neg7(2)	0.0095	125.498	10.782	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(2)	2(1)					
1S	2.27(2)	3(1)					
1S	2.38(2)	2(1)					
1Br	2.33(4)	9(4)					
1Imd	1.96(2)	4(1)	neg7(2)	0.0093	123.168	10.582	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.12(1)	2(1)					
1S	2.33(1)	0(1)					
1S	1.65(3)	25(4)					
1Br	1.99(1)	9(1)					
1Imd	1.97(2)	4(2)	neg5(1)	0.0105	138.796	11.924	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(2)	1(2)					
2S	2.30(8)	4(1)					
1Br	2.06(6)	19(8)					
1Imd	1.96(2)	4(2)	neg7(1)	0.0145	191.310	14.026	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Br	2.18(0.20)	37(39)					
1Imd	1.98(2)	3(1)	neg6(1)	0.0146	193.377	14.178	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Br	2.13(0.15)	32(2)					
1Imd	1.97(2)	3(1)	neg7(1)	0.0153	202.384	14.838	9

Zn-N(2.0) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	0(1)					
2S	2.30(1)	3(0)					
1Br	2.20(0.20)	37(37)					
1Imd	1.97(2)	3(1)	neg7(1)	0.0151	200.228	14.680	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	0(1)					
2S	2.31(1)	3(1)					
1Br	2.34(6)	19(10)					
1Imd	1.98(2)	3(1)	neg7(1)	0.0164	216.498	15.873	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	0(1)					
2S	2.31(1)	3(1)					
1Br	2.34(6)	30(10)					
1Imd	1.98(2)	3(1)	neg7(1)	0.0159	209.809	15.382	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	0(1)					
2S	2.31(1)	3(1)					
1Br	2.34(5)	17(8)					
1Imd	1.97(2)	3(1)	neg7(1)	0.0168	221.759	16.258	9

Zn-N(2.0) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(2)	0(1)					
2S	2.31(1)	3(1)					
1Br	2.34(5)	18(8)					
1Imd	1.98(2)	3(1)	neg7(1)	0.0162	215.093	15.770	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.10(1)	2(1)					
1S	2.32(1)	0(1)					
2Br	2.02(3)	18(4)					
1Imd	1.98(2)	3(2)	neg4(2)	0.0289	382.635	28.053	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
2Br	2.50(7)	23(8)					
1Imd	1.99(3)	2(2)	neg5(2)	0.0487	645.083	47.295	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
2Br	2.49(7)	23(9)					
1Imd	1.99(3)	2(2)	neg5(2)	0.0489	646.685	47.412	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
2Br	2.50(7)	24(8)					
1Imd	2.00(3)	2(2)	neg4(2)	0.0481	636.514	46.666	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
2Br	2.50(8)	25(10)					
1Imd	1.99(3)	2(2)	neg5(2)	0.0496	656.560	48.136	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
2Br	2.50(8)	26(11)					
1Imd	1.99(3)	2(2)	neg5(2)	0.0497	657.826	48.229	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.32(1)	0(1)					
2Br	2.51(8)	25(10)					
1Imd	2.00(3)	2(2)	neg4(2)	0.0487	645.213	47.304	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.32(1)	0(1)					
2Br	2.51(9)	27(12)					
1Imd	2.00(3)	2(2)	neg4(2)	0.0502	664.410	48.712	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.31(1)	0(1)					
2Br	2.51(0.10)	28(13)					
1Imd	1.99(3)	2(2)	neg5(2)	0.0503	665.326	48.779	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.32(1)	0(1)					
2Br	2.52(8)	27(11)					
1Imd	2.00(3)	2(2)	neg3(2)	0.0492	651.266	47.748	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.09(2)	2(1)					
1S	2.32(1)	0(1)					
2Br	2.52(0.10)	29(14)					
1Imd	2.00(3)	2(2)	neg4(2)	0.0506	669.679	49.098	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.15(3)	2(2)					
1S	2.57(2)	3(2)					
2Br	2.51(2)	4(2)					
1Imd	2.11(6)	3(5)	neg5(3)	0.2129	2818.384	2818.384	9

Table K.7. Additional Fits for Zn(II) C201A-PHD2 in Buffer with 50 mM PBS, 150 mM NaBr at pH 7.2.
Data Fit from k = 2 - 12.5 Å^{-1} and R = 1- 2.5 Å.

Ni-N(2.0)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(3)	1.1(1.8)	7.7(5.7)	0.2944	3159.383	385.144	3
3N/O	2.15(2)	2.8(1.3)	6.6(3.4)	0.1721	1846.599	225.109	3
4N/O	2.15(2)	4.2(1.1)	5.6(2.3)	0.1088	1167.704	142.349	3
5N/O	2.15(1)	5.5(1.0)	4.7(1.9)	0.0846	907.944	110.683	3
6N/O	2.14(1)	6.9(1.1)	3.9(1.8)	0.0864	926.839	112.986	3
7N/O	2.14(2)	8.3(1.3)	3.1(1.9)	0.1049	1125.426	137.195	3

Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.25(2)	4.5(1.2)	11.3(5.3)	0.1689	1813.101	221.0260	3
3S	2.25(2)	6.7(0.9)	12.4(3.4)	0.0916	982.554	119.7780	3
4S	2.25(1)	8.6(0.8)	13.3(2.7)	0.0642	689.465	84.0490	3
5S	2.25(1)	10.4(0.8)	14.0(2.5)	0.0622	668.017	81.4340	3
6S	2.25(2)	12.0(1.0)	14.6(2.7)	0.0733	787.071	95.9480	3
7S	2.25(2)	13.6(1.1)	15.1(3.0)	0.0911	977.342	119.1430	3

Ni-N(2.0) Ni-N(2.2)

N	Radius Å	σ^2(x10^{-3} Å^2)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.09(2)	1.5(1.2)					
1N/O	2.21(2)	4.3(1.1)	4.4(2.6)	0.0779	835.684	134.720	5
2N/O	2.07(1)	0.6(1.1)					
2N/O	2.19(1)	1.8(0.9)	3.1(1.7)	0.0436	467.872	75.425	5
3N/O	2.10(1)	1.1(1.0)					
1N/O	2.21(1)	3.2(1.0)	3.5(1.7)	0.0436	468.124	75.466	5
4N/O	2.10(1)	3.5(1.2)					
1N/O	2.21(1)	2.2(1.1)	2.6(1.6)	0.0403	432.229	69.679	5
3N/O	2.08(1)	2.1(1.3)					
2N/O	2.19(1)	0.7(1.1)	2.2(1.6)	0.0436	468.401	75.511	5
5N/O	2.10(2)	5.8(1.6)					
1N/O	2.20(2)	1.3(1.5)	1.8(1.8)	0.0542	581.608	93.761	5
4N/O	2.08(2)	5.0(2.1)					
2N/O	2.19(2)	0.5(1.6)	1.4(1.9)	0.0596	639.879	103.154	5
3N/O	2.05(2)	3.9(2.4)					
3N/O	2.18(2)	1.5(1.6)	1.0(1.9)	0.0651	698.524	112.608	5

6N/O	2.1(2)	8.3(2.3)					
1N/O	2.19(2)	0.5(1.9)	1.1(2.1)	0.0764	820.082	132.205	5
5N/O	2.08(3)	8.6(3.4)					
2N/O	2.18(2)	1.6(2.0)	0.6(2.3)	0.0810	869.773	140.215	5
4N/O	2.06(4)	8.8(5.0)					
3N/O	2.17(2)	3.0(2.1)	0.2(2.4)	0.0859	921.452	148.546	5

Ni-S(2.2) Ni-S(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.19(2)	3.8(1.6)					
1S	2.30(2)	0.7(1.5)	15.2(3.7)	0.0637	683.823	110.238	5
2S	2.17(3)	5.7(2.3)					
2S	2.28(2)	3.7(1.7)	16.3(3.3)	0.0497	533.565	86.016	5
3S	2.26(2)	4.7(1.3)					
1S	2.13(3)	3.2(2.2)	15.6(3.3)	0.0526	564.404	90.987	5
4S							
1S			No Fit	No Fit	No Fit	No Fit	5
3S	2.27(2)	5.8(2.2)					
2S	2.15(4)	8.1(4.3)	17.0(3.5)	0.0520	558.409	90.021	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.26(2)	8.1(1.0)					
2S	2.48(6)	18.3(11.1)	9.5(3.1)	0.0458	491.750	79.275	5
3S	2.16(6)	15.4(8.2)					
3S	2.25(2)	7.1(1.9)	18.1(4.0)	0.0538	577.611	93.116	5
6S	2.23(2)	10.3(1.4)					
1S	2.03(5)	10.8(7.8)	17.6(3.6)	0.0609	653.826	105.403	5
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.27(1)	8.0(0.9)					
3S	2.49(4)	20.9(8.3)	8.6(2.7)	0.0382	410.074	66.108	5

Ni-N(2.0) Ni-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	1.8(1.5)					5
1S	2.30(2)	1.1(1.1)	3.9(3.7)	0.0690	740.384	119.357	

1N/O 2S			No Fit	No Fit	No Fit	No Fit	5
2N/O 2S	2.04(3) 2.28(2)	4.8(2.3) 4.6(1.1)	8.2(3.3)	0.0513	550.032	88.670	5
3N/O 1S	2.08(2) 2.31(2)	4.4(1.4) 1.9(1.1)	2.8(2.8)	0.0425	456.228	73.548	5
1N/O 3S			No Fit	No Fit	No Fit	No Fit	5
1N/O 4S	1.95(0.12) 2.25(2)	10.7(12.2) 8.5(1.2)	13.6(3.8)	0.0549	589.303	95.001	5
4N/O 1S	2.09(2) 2.31(1)	6.9(1.4) 2.8(1.2)	1.9(2.5)	0.0323	346.529	55.864	5
2N/O 3S	2.01(7) 2.26(2)	10.1(5.5) 7.0(1.2)	11.1(4.0)	0.0520	557.975	89.951	5
3N/O 2S	2.05(4) 2.28(2)	8.3(2.7) 5.3(1.3)	7.2(3.7)	0.0468	501.908	80.912	5
5N/O 1S	2.11(3) 2.30(1)	9.4(1.5) 3.5(1.3)	0.7(2.6)	0.0286	306.917	49.478	5
1N/O 5S			No Fit	No Fit	No Fit	No Fit	5
4N/O 2S	2.08(5) 2.28(2)	11.4(3.4) 5.9(1.5)	5.8(4.3)	0.0448	481.322	77.593	5
2N/O 4S			No Fit	No Fit	No Fit	No Fit	5
3N/O 3S	2.03(0.1) 2.26(2)	15.7(7.0) 7.3(1.3)	10.6(4.7)	0.0516	554.232	89.347	5
6N/O 1S	2.13(3) 2.29(1)	11.4(1.8) 3.8(1.4)	0.5(2.6)	0.0274	294.452	47.468	5
1N/O 6S	1.79(0.1) 2.24(2)	14.1(16.1) 11.7(1.1)	15.9(3.3)	0.0669	717.854	115.725	5
5N/O 2S	2.11(6) 2.28(2)	13.3(4.7) 6.4(1.9)	3.8(5.0)	0.0426	457.086	73.686	5
2N/O			No Fit	No Fit	No Fit	No Fit	5

5S							
4N/O	2.05(0.11)	20.1(8.2)					
3S	2.26(2)	7.4(1.3)	10.0(5.4)	0.0513	550.222	88.701	5
3N/O	1.96(0.21)	29.0(22.6)					
4S	2.25(2)	8.7(1.1)	13.6(5.0)	0.0538	577.802	93.147	5

Table K.8. Additional Fits for Zn(II) C201A-PHD2 in Buffer with 50 mM PBS, 150 mM NaBr at pH 7.2.
Data Fit from k = 2 - 12.5 $Å^{-1}$ and R = 1- 4 Å.

Zn-N(2.0)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.16(2)	1(1)	8(4)	0.3435	3946.120	200.926	3
3N/O	2.15(1)	3(1)	7(3)	0.2273	2611.555	132.974	3
4N/O	2.15(1)	4(1)	6(2)	0.1671	1919.293	97.725	3
5N/O	2.15(1)	6(1)	5(2)	0.1438	1652.462	84.139	3
6N/O	2.14(1)	7(1)	4(2)	0.1452	1668.663	84.964	3
7N/O	2.14(1)	8(1)	3(2)	0.1625	1867.212	95.074	3

Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} $Å^2$)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2S	2.25(2)	5(01)	11(4)	0.2191	2517.062	128.162	3
3S	2.25(1)	7(1)	12(3)	0.1451	1667.430	84.901	3
4S	2.25(1)	9(1)	13(2)	0.1189	1366.518	69.580	3
5S	2.25(1)	10(1)	14(2)	0.1169	1342.686	68.366	3
6S	2.25(1)	12(1)	15(2)	0.1273	1462.012	74.442	3
7S	2.25(2)	14(1)	15(3)	0.1440	1653.854	84.210	3

Zn-N(2.0) Zn-N(2.2)

	r(Å)	σ^2(x10^{-3} $Å^2$)	ΔE_o(eV)	R factor	Reduced χ^2	χ^2	nvar
2N/O	2.10(1)	1(1)					
1N/O	2.22(1)	4(1)	5(2)	0.1362	1564.988	88.720	5
2N/O	2.07(1)	1(1)					
2N/O	2.19(1)	2(1)	3(2)	0.1013	1163.325	65.949	5
3N/O	2.10(1)	1(1)					
1N/O	2.22(1)	3(1)	4(2)	0.1038	1192.027	67.577	5
4N/O	2.10(1)	4(1)					
1N/O	2.21(1)	2(1)	3(2)	0.1007	1156.510	65.563	5

3N/O	2.08(1)	2(1)					
2N/O	2.20(1)	1(1)	2(2)	0.1021	1173.248	66.512	5
5N/O	2.10(1)	6(1)					
1N/O	2.20(2)	1(1)	2(2)	0.1141	1310.438	74.289	5
4N/O	2.08(2)	5(2)					
2N/O	2.19(1)	1(1)	2(2)	0.1178	1353.294	76.719	5
3N/O	2.06(2)	4(2)					
3N/O	2.18(1)	2(1)	1(2)	0.1215	1395.561	79.115	5
6N/O	2.10(2)	8(2)					
1N/O	2.19(2)	0(2)	1(2)	0.1354	1555.627	88.189	5
5N/O	2.08(2)	9(3)					
2N/O	2.18(2)	2(2)	1(2)	0.1385	1591.473	90.221	5
4N/O	2.06(3)	9(4)					
3N/O	2.17(2)	3(2)	0(2)	0.1422	1633.348	92.595	5

Zn-S(2.2) Zn-S(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2S	2.19(2)	4(1)					
1S	2.31(2)	1(1)	15(3)	0.1147	1317.363	74.682	5
2S	2.17(2)	6(2)					
2S	2.28(2)	4(1)	16(3)	0.1036	1190.378	67.483	5
3S	2.26(2)	5(1)					
1S	2.13(2)	3(2)	15(3)	0.1067	1225.536	69.476	5
4S	2.26(2)	8(1)					
1S	2.50(7)	13(11)	11(3)	0.1096	1259.520	71.410	5
3S	2.27(2)	6(2)					
2S	2.15(3)	2(4)	17(3)	0.1070	1229.520	69.702	5
5S							
1S			No Fit	No Fit	No Fit	No Fit	5
4S	2.26(1)	8(1)					
2S	2.48(5)	19(10)	10(3)	0.1016	1167.426	66.182	5
3S	2.16(5)	15(7)					
3S	2.25(2)	7(2)	18(4)	0.1088	1250.446	70.888	5
6S			No Fit	No Fit	No Fit	No Fit	5

1S							
5S							
2S			No Fit	No Fit	No Fit	No Fit	5
4S	2.27(1)	8(1)					
3S	2.49(4)	21(8)	9(3)	0.0942	1082.525	61.369	5

Zn-N(2.0) Zn-S(2.2)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	2(1)					5
1S	2.30(1)	1(1)	4(3)	0.1221	1403.333	79.556	
1N/O							5
2S			No Fit	No Fit	No Fit	No Fit	
2N/O	2.04(3)	5(2)					
2S	2.28(1)	5(1)	8(3)	0.1063	1221.171	69.229	5
3N/O	2.08(2)	4(1)					
1S	2.31(1)	2(1)	3(3)	0.0981	1126.723	63.874	5
1N/O							
3S			No Fit	No Fit	No Fit	No Fit	5
1N/O	1.95(0.10)	11(10)					
4S	2.25(2)	9(1)	14(3)	0.1100	1263.922	71.652	5
4N/O	2.09(2)	7(1)					
1S	2.31(1)	3(1)	2(3)	0.0895	1028.179	58.288	5
2N/O	2.01(6)	10(5)					
3S	2.26(2)	7(1)	11(3)	0.1074	1233.502	69.928	5
3N/O	2.05(4)	8(2)					
2S	2.28(2)	5(1)	7(3)	0.1026	1178.547	66.812	5
5N/O	2.11(3)	9(2)					
1S	2.30(1)	4(1)	1(3)	0.0870	999.199	56.645	5
1N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.08(5)	12(3)					
2S	2.28(2)	6(1)	6(4)	0.1011	1161.628	65.853	5
2N/O							
4S			No Fit	No Fit	No Fit	No Fit	5

3N/O	2.03(9)	16(6)					
3S	2.26(2)	7(1)	11(4)	0.1071	1230.953	69.783	5
6N/O	2.13(3)	12(2)					
1S	2.30(1)	4(1)	0(3)	0.0867	996.245	56.478	5
1N/O	1.79(8)	14(13)					
6S	2.24(2)	12(1)	16(3)	0.1213	1393.304	78.987	5
5N/O	2.11(6)	14(4)					
2S	2.28(1)	6(2)	4(5)	0.0993	1140.811	64.673	5
2N/O							
5S			No Fit	No Fit	No Fit	No Fit	5
4N/O	2.05(0.1)	20(7)					
3S	2.26(2)	7(1)	10(5)	0.1068	1226.793	69.547	5
3N/O	1.97(0.19)	29(19)					
4S	2.25(2)	9(1)	14(4)	0.1091	1253.719	71.074	5

Zn-N(2.0) Zn-Br(2.3)

N	**Radius Å**	**σ^2 (x10^{-3} Å^2)**	**ΔE_0 (eV)**	**R factor**	**χ^2**	**Red χ^2**	**nvar**
2N/O	2.13(2)	2(1)					5
1Br	2.45(3)	7(2)	4(4)	0.2482	2851.693	161.664	
1N/O	1.93(6)	3(4)					5
2Br	2.31(3)	7(1)	neg34(9)	0.3277	3764.954	213.437	
2N/O	2.14(2)	2(1)					
2Br	2.47(3)	13(3)	5(4)	0.2518	2892.407	163.972	5
3N/O	2.14(2)	3(1)					
1Br	2.45(2)	8(2)	4(3)	0.1540	1769.469	100.312	5
1N/O	1.89(6)	5(6)					
3Br	2.30(3)	9(1)	neg37(8)	0.2748	3156.607	178.950	5
1N/O	1.86(6)	6(6)					
4Br	2.29(3)	11(10)	neg39(7)	0.2415	2775.038	157.318	5
4N/O	2.14(1)	5(1)					
1Br	2.45(2)	9(2)	4(2)	0.1036	1189.909	67.456	5
2N/O	2.15(2)	2(1)					
3Br	2.48(3)	16(3)	5(4)	0.2552	2931.786	166.204	5
3N/O	2.15(2)	4(1)					
2Br	2.47(2)	14(3)	5(3)	0.1574	1808.382	102.518	5

5N/O	2.14(1)	7(1)					
1Br	2.44(2)	9(2)	4(2)	0.0816	937.767	53.162	5
1N/O	2.87(4)	0(3)					
5Br	2.29(2)	12(1)	neg40(6)	0.2340	2688.596	152.418	5
4N/O	2.15(1)	5(1)					
2Br	2.46(2)	14(2)	5(2)	0.1064	1222.762	69.319	5
2N/O	2.15(2)	2(1)					
4Br	2.49(4)	19(3)	5(4)	0.2594	2979.995	168.937	5
3N/O	2.15(2)	4(1)					
3Br	2.47(3)	17(3)	5(3)	0.1609	1848.493	104.792	5
6N/O	2.14(1)	8(1)					
1Br	2.43(1)	9(2)	3(1)	0.0779	895.164	50.747	5
1N/O							
6Br			No Fit	No Fit	No Fit	No Fit	5
5N/O	2.15(1)	7(1)					
2Br	2.45(2)	14(2)	4(1)	0.0839	964.366	54.670	5
2N/O	2.15(2)	2(1)					
5Br	2.49(4)	21(4)	6(4)	0.2640	3032.560	171.917	5
4N/O	2.15(1)	5(1)					
3Br	2.46(2)	18(3)	5(2)	0.1095	1258.155	71.325	5
3N/O	2.15(2)	3(1)					
4Br	2.48(3)	20(3)	5(2)	0.1649	1894.712	107.412	5

Zn-N(2.0) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
5N/O	2.14(1)	4(1)					
1Imd	1.99(1)	0(1)	2(1)	0.0778	893.501	50.653	5
4N/O	2.14(1)	3(1)					
1Imd	2.00(1)	0(1)					
1Imd	2.18(3)	2(2)	3(1)	0.0618	709.978	45.396	7
3N/O	2.14(1)	2(1)					
1Imd	1.94(3)	1(4)					
1Imd	2.18(2)	2(2)					
1Imd	2.04(2)	3(2)	0(1)	0.0535	614.507	45.053	9
2N/O	2.14(1)	0(1)	2(3)	0.0730	838.159	72.009	11

1Imd	2.09(6)	3(6)					
1Imd	2.45(0.15)	14(26)					
1Imd	1.98(5)	1(6)					
1Imd	2.21(4)	3(3)					
1N/O	2.15(2)	3(2)					
1Imd	2.34(6)	9(4)					
1Imd	2.52(6)	3(6)					
1Imd	2.10(4)	11(3)					
1Imd	2.22(5)	12(3)					
1Imd	2.00(4)	7(3)	5(3)	0.1040	1195.099	123.977	13
4N/O	2.15(1)	2(1)					
1Imd	2.01(1)	0(1)	3(1)	0.0869	998.930	56.630	5
3N/O	2.14(1)	2(1)					
1Imd	2.02(1)	1(1)					
1Imd	2.19(2)	0(2)	3(1)	0.0659	757.010	48.403	7
2N/O	2.14(1)	0(1)					
1Imd	2.2(2)	4(2)					
1Imd	1.97(3)	1(4)					
1Imd	2.07(3)	4(3)	2(2)	0.0858	985.190	72.230	9
1N/O	2.13(2)	3(2)					
1Imd	2.16(3)	11(3)					
1Imd	2.05(3)	10(3)					
1Imd	2.26(3)	8(4)					
1Imd	1.95(3)	6(3)	2(2)	0.1345	1545.267	132.759	11
0N/O							
1Imd							
1Imd							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
3N/O	2.15(1)	1(1)					
1Imd	2.02(2)	0(1)	3(2)	0.1339	1537.961	87.188	5
2N/O	2.14(1)	0(1)					
1Imd	2.03(2)	1(1)					
1Imd	2.19(2)	1(1)	4(2)	0.1012	1162.994	74.362	7
1N/O							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
0N/O			3(3)	0.3048	3501.265	256.698	9

1Imd	2.22(0.74)	3(77)					
1Imd	2.08(0.16)	7(12)					
1Imd	2.18(0.61)	6(22)					
1Imd	1.98(5)	5(8)					
2N/O	2.16(2)	0(1)					
1Imd	2.04(2)	0(2)	4(3)	0.2356	2706.292	153.421	5
1N/O	2.14(2)	2(2)					
1Imd	2.19(2)	3(1)					
1Imd	2.05(2)	2(1)	5(2)	0.1855	2131.190	136.268	7
0N/O							
1Imd	2.00(3)	5(3)					
1Imd	2.22(2)	7(2)					
1Imd	2.11(2)	8(3)	No Fit	No Fit	No Fit	No Fit	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	2(2)					
1S	2.31(2)	1(1)					
1Br	2.34(0.13)	20(21)	neg3(3)	0.1191	1368.753	87.518	7
1N/O	2.04(3)	0(2)					
2S	2.29(3)	4(2)					
1Br	2.30(0.10)	14(14)	neg8(4)	0.1171	1345.135	86.008	7
1N/O	2.05(3)	1(2)					
1S	2.29(2)	1(1)					
2Br	2.44(0.11)	23(15)	neg6(5)	0.1779	2043.942	130.690	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(2)	2(2)					
1S	2.31(2)	1(1)					
1Br	2.35(0.12)	20(18)	neg3(3)	0.1169	1343.458	85.901	7
1N/O	2.04(3)	0(2)					
2S	2.29(3)	4(2)					
1Br	2.31(0.10)	14(13)	neg8(4)	0.1149	1319.902	84.395	7
1N/O	2.05(3)	1(2)					
1S	2.29(2)	1(1)					
2Br	2.43(0.11)	25(18)	neg6(5)	0.1771	2034.278	130.072	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar

2N/O	2.07(2)	2(2)					
1S	2.31(2)	1(1)					
1Br	2.33(0.15)	21(24)	neg4(4)	0.1246	1431.744	91.546	7
1N/O	2.04(3)	1(2)					
2S	2.29(4)	4(2)					
1Br	2.30(0.10)	12(13)	neg9(4)	0.1167	1341.088	85.749	7
1N/O	2.04(3)	1(2)					
1S	2.28(2)	1(1)					
2Br	2.43(0.11)	22(14)	neg8(6)	0.1800	2067.848	132.218	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	2(2)					
1S	2.31(2)	1(1)					
1Br	2.34(0.13)	20(20)	neg4(4)	0.1224	1405.758	89.884	7
1N/O	2.04(3)	1(2)					
2S	2.29(3)	4(2)					
1Br	2.30(9)	13(12)	neg9(4)	0.1147	1317.936	84.269	7
1N/O	2.05(3)	1(2)					
1S	2.29(2)	1(1)					
2Br	2.42(0.11)	25(18)	neg7(5)	0.1800	2068.056	132.232	7

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(3)	2(2)					
1S	2.31(2)	1(1)					
1Br	2.33(0.17)	22(25)	neg5(4)	0.1278	1467.833	93.853	7
1N/O	2.03(3)	1(3)					
2S	2.29(4)	4(2)					
1Br	2.30(0.10)	11(12)	neg10(4)	0.1150	1321.499	84.497	7
1N/O	2.04(3)	0(2)					
1S	2.28(2)	1(1)					
2Br	2.43(0.10)	21(13)	neg9(6)	0.1797	2063.973	131.971	7

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.07(2)	2(2)					
1S	2.31(2)	1(1)					
1Br	2.33(0.14)	20(21)	neg5(4)	0.1255	1441.966	92.199	7

1N/O	2.03(3)	1(2)					
2S	2.29(4)	4(2)					
1Br	2.30(9)	12(12)	neg10(4)	0.1132	1300.379	83.146	7
1N/O	2.04(3)	1(2)					
1S	2.29(2)	1(1)					
2Br	2.42(0.11)	24(17)	neg8(6)	0.1803	2071.294	132.439	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	4(2)					
1S	2.33(3)	2(2)					
1Br	2.34(7)	14(10)	neg1(3)	0.0883	1014.844	64.889	7
2N/O	2.07(2)	4(2)					
2S	2.34(5)	5(3)					
1Br	2.35(6)	7(4)	neg4(3)	0.0887	1018.836	65.144	7
1N/O							
3S							
1Br			No Fit	No Fit	No Fit	No Fit	7
2N/O	2.08(2)	1(1)					
1S	2.31(2)	1(1)					
2Br	2.34(0.12)	27(19)	neg3(3)	0.1187	1363.397	87.176	7
1N/O	2.35(0.20)	2(15)					
1S	2.08(8)	5(4)					
3Br	2.32(6)	10(6)	neg37(11)	0.1859	2135.876	136.568	7

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	4(1)					
1S	2.33(2)	2(1)					
1Br	2.35(6)	15(9)	neg1(3)	0.0866	994.771	63.606	7
2N/O	2.07(2)	4(2)					
2S	2.33(4)	5(3)					
1Br	2.35(5)	8(4)	neg4(3)	0.0875	1005.627	64.300	7
1N/O	2.03(3)	2(2)					
3S	2.31(3)	6(2)					
1Br	2.33(5)	8(4)	neg7(3)	0.0878	1008.650	64.493	7
2N/O	2.08(2)	1(1)					
1S	2.31(2)	1(1)					
2Br	2.35(0.10)	26(15)	neg3(3)	0.1152	1323.108	84.600	7

1N/O	2.06(2)	1(2)					
1S	2.29(2)	1(1)					
3Br	2.42(0.13)	33(25)	neg5(5)	0.1789	2055.785	131.447	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(2)	4(2)					
1S	2.33(3)	2(2)					
1Br	2.33(7)	13(10)	neg2(3)	0.0933	1072.173	68.555	7
2N/O	2.06(2)	4(2)					
2S	2.34(5)	5(4)					
1Br	2.35(6)	6(3)	neg5(4)	0.0899	1032.680	66.030	7
1N/O	2.02(3)	2(3)					
3S	2.31(4)	7(3)					
1Br	2.33(5)	7(3)	neg9(4)	0.0896	1029.329	65.815	7
2N/O	2.06(2)	2(2)					
1S	2.30(2)	1(1)					
2Br	2.20(0.34)	42(72)	neg5(4)	0.1240	1424.338	91.072	7
1N/O	2.06(3)	1(2)					
1S	2.29(2)	1(1)					
3Br	1.94(6)	23(7)	neg9(5)	0.1498	1720.760	110.025	7

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(2)	4(2)					
1S	2.33(3)	2(1)					
1Br	2.34(7)	14(9)	neg2(3)	0.0914	1050.038	67.139	7
2N/O	2.06(2)	4(2)					
2S	2.34(5)	5(3)					
1Br	2.35(6)	7(4)	neg5(3)	0.0888	1019.845	65.209	7
1N/O	2.02(3)	2(2)					
3S	2.31(3)	7(3)					
1Br	2.33(5)	7(3)	neg9(3)	0.0874	1004.050	64.199	7
2N/O	2.07(2)	1(1)					
1S	2.31(2)	1(1)					
2Br	2.33(0.11)	27(17)	neg4(3)	0.1206	1386.054	88.624	7
1N/O	2.05(3)	1(2)					
1S	2.29(2)	1(1)	neg7(5)	0.1823	2094.389	133.915	7

3Br	2.41(0.15)	33(29)					

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.10(2)	4(1)					
1S	2.39(8)	4(7)					
1Br	2.39(6)	6(3)	neg1(3)	0.0968	1112.494	71.133	7
2N/O	2.06(2)	4(2)					
2S	2.34(5)	5(4)					
1Br	2.35(6)	6(3)	neg6(4)	0.0904	1038.815	66.422	7
1N/O	1.33(0.21)	23(36)					
3S	2.26(3)	7(3)					
1Br	2.32(8)	12(11)	neg14(4)	0.1190	1367.681	87.450	7
2N/O	2.06(2)	2(2)					
1S	2.30(2)	1(1)					
2Br	2.18(0.34)	42(82)	neg6(4)	0.1267	1455.919	93.092	7
1N/O							
1S							
3Br			No Fit	No Fit	No Fit	No Fit	7

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5)

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(2)	4(2)					
1S	2.33(3)	2(2)					
1Br	2.34(7)	14(9)	neg3(3)	0.0950	1091.178	69.770	7
2N/O	2.06(2)	4(2)					
2S	2.34(5)	5(3)					
1Br	2.35(5)	6(3)	neg6(4)	0.0892	1024.973	65.537	7
1N/O	2.02(3)	3(3)					
3S	2.31(3)	7(3)					
1Br	2.33(4)	7(3)	neg10(3)	0.0864	992.627	63.469	7
2N/O	2.07(2)	2(1)					
1S	2.31(2)	1(1)					
2Br	2.32(0.12)	27(18)	neg5(3)	0.1238	1422.514	90.956	7
1N/O	2.12(2)	2(1)					
1S	2.57(2)	2(1)					
3Br	2.51(2)	7(2)	6(4)	0.2499	2871.625	183.612	7

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	2(1)					
1S	2.31(1)	2(1)					
1Imd	1.95(1)	1(1)	neg4(1)	0.0335	384.632	24.593	7
2N/O	2.07(2)	1(1)					
2S	2.30(1)	5(1)					
1Imd	1.94(2)	1(1)	neg7(2)	0.0509	584.646	37.382	7
2N/O	2.08(1)	1(1)					
1S	2.31(1)	1(1)					
1Imd	1.91(9)	22(19)					
1Imd	1.95(1)	0(1)	neg6(1)	0.0287	329.880	24.185	9
1N/O							
2S							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.08(1)	3(1)					
1S	2.30(1)	0(1)					
1Imd	1.96(2)	0(1)					
1Imd	1.95(0.21)	20(39)					
1Imd	2.13(8)	5(8)	neg5(3)	0.0493	566.221	48.646	11
0N/O							
2S							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-S(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	2(1)					
1S	2.32(1)	2(1)					
1Imd	1.95(1)	1(1)	neg4(1)	0.0351	403.297	25.787	7
2N/O	2.07(2)	1(1)					
2S	2.29(1)	5(1)					
1Imd	1.94(2)	1(1)	neg8(2)	0.0543	623.478	39.865	7
2N/O	2.08(1)	1(1)					
1S	2.31(1)	1(1)					
1Imd	1.95(1)	0(1)					
1Imd	1.90(8)	21(18)	neg6(2)	0.0306	352.032	25.809	9
1N/O	2.05(1)	2(1)	neg10(2)	0.0424	487.659	35.753	9

2S	2.28(1)	4(1)					
1Imd	1.94(1)	0(1)					
1Imd	1.81(4)	12(7)					
1N/O	2.07(1)	3(1)					
1S	2.30(1)	1(1)					
1Imd	1.92(0.17)	18(31)					
1Imd	2.12(8)	4(7)					
1Imd	1.96(2)	0(2)	neg5(3)	0.0526	604.549	51.939	11
0N/O							
2S	2.27(2)	4(1)					
1Imd	1.99(5)	0(4)					
1Imd	2.14(0.14)	5(13)					
1Imd	1.88(0.10)	6(9)	neg10(4)	0.1331	1529.339	112.124	9

Zn-N(2.0) Zn-S(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	2(1)					
1S	2.32(1)	2(1)					
1Imd	1.95(2)	1(1)	neg5(1)	0.0366	420.234	26.870	7
2N/O	2.07(2)	1(1)					
2S	2.29(1)	5(1)					
1Imd	1.94(2)	1(1)	neg8(2)	0.0570	655.137	41.890	7
2N/O	2.08(1)	1(1)					
1S	2.31(1)	1(1)					
1Imd	1.95(1)	0(1)					
1Imd	1.89(7)	20(16)	neg7(2)	0.0321	368.654	27.028	9
1N/O	2.05(1)	2(1)					
2S	2.28(1)	4(1)					
1Imd	1.94(1)	0(1)					
1Imd	1.81(4)	12(7)	neg11(2)	0.0439	504.176	36.964	9
1N/O	2.07(1)	3(1)					
1S	2.30(1)	1(1)					
1Imd	1.91(0.15)	16(25)					
1Imd	2.12(8)	4(7)					
1Imd	1.96(3)	0(2)	neg6(3)	0.0551	632.885	54.373	11
0N/O							
2S	2.26(2)	4(1)					
1Imd	1.66(0.17)	17(24)					
1Imd	1.85(7)	5(9)					
1Imd	1.98(4)	0(4)	neg13(4)	0.1336	1535.125	112.549	9

Zn-N(2.0) Zn-S(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	2(1)					
1S	2.32(1)	2(1)					
1Imd	1.95(2)	1(1)	neg5(1)	0.0379	435.533	27.848	7
2N/O	2.07(2)	1(1)					
2S	2.29(1)	5(1)					
1Imd	1.93(2)	2(1)	neg9(2)	0.0590	678.152	43.361	7
2N/O	2.07(1)	1(1)					
1S	2.31(1)	1(1)					
1Imd	1.95(1)	0(1)					
1Imd	1.88(7)	19(15)	neg7(2)	0.0334	383.676	28.129	9
1N/O	2.05(1)	2(1)					
2S	2.28(1)	4(1)					
1Imd	1.80(4)	11(6)					
1Imd	1.93(1)	0(1)	neg11(2)	0.0450	516.981	37.903	9
1N/O	2.07(1)	3(1)					
1S	2.30(1)	1(1)					
1Imd	1.96(3)	0(2)					
1Imd	1.89(0.14)	16(23)					
1Imd	2.11(8)	4(7)	neg6(3)	0.0575	660.064	56.708	11
0N/O							
2S	2.26(2)	4(1)					
1Imd	1.99(5)	0(3)					
1Imd	2.14(0.14)	6(13)					
1Imd	1.86(9)	5(8)	neg12(4)	0.1354	1555.800	114.065	9

Zn-N(2.0) Zn-S(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.16(1)	1(1)					
1S	2.71(5)	11(6)					
1Imd	2.02(2)	0(1)	4(2)	0.1294	1486.112	95.022	7
2N/O	2.07(2)	2(1)					
2S	2.29(1)	5(1)					
1Imd	1.93(2)	2(2)	neg9(2)	0.0609	699.575	44.731	7
2N/O	2.14(1)	0(1)					
1S	2.71(3)	8(4)					
1Imd	2.20(2)	2(1)					
1Imd	2.04(2)	2(1)	4(1)	0.0865	993.502	72.839	9
1N/O	2.05(1)	2(1)	neg10(2)	0.0479	550.159	40.335	9

2S	2.29(1)	4(1)					
1Imd	2.75(5)	6(5)					
1Imd	1.94(1)	0(1)					
1N/O	2.14(2)	2(2)					
1S	2.70(5)	8(6)					
1Imd	2.22(0.14)	2(15)					
1Imd	2.13(0.10)	2(36)					
1Imd	2.02(0.12)	2(12)	4(2)	0.1457	1674.200	143.836	11
0N/O							
2S	2.26(2)	4(1)					
1Imd	1.86(9)	5(8)					
1Imd	1.99(5)	0(3)					
1Imd	2.15(0.14)	6(14)	neg13(4)	0.1345	1544.998	113.273	9

Zn-N(2.0) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(1)	1(1)					
1Br	2.45(2)	9(2)					
1Imd	2.01(2)	0(1)	1(2)	0.0797	915.235	58.520	7
2N/O	2.15(2)	0(1)					
2Br	2.46(3)	13(3)					
1Imd	2.02(3)	0(2)	1(3)	0.1680	1929.873	123.396	7
2N/O	2.13(1)	0(1)					
1Br	2.46(2)	10(2)					
1Imd	2.02(2)	1(1)					
1Imd	2.19(2)	0(1)	3(2)	0.0640	735.602	53.931	9
1N/O	2.13(2)	2(2)					
2Br	2.47(3)	14(3)					
1Imd	2.04(2)	2(2)					
1Imd	2.19(2)	2(1)	3(2)	0.1417	1628.188	119.372	9
1N/O	2.13(2)	2(1)					
1Br	2.46(3)	9(3)					
1Imd	2.16(5)	3(6)					
1Imd	2.02(3)	3(3)					
1Imd	2.25(9)	2(16)	4(2)	0.1091	1253.302	107.675	11
0N/O							
2Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(1)	1(1)					
1Br	2.45(2)	9(2)					
1Imd	2.01(2)	0(1)	1(2)	0.0808	928.614	59.376	7
2N/O	2.15(2)	0(1)					
2Br	2.46(3)	13(3)					
1Imd	2.03(3)	0(2)	2(3)	0.1699	1952.018	124.812	7
2N/O	2.13(1)	0(1)					
1Br	2.46(2)	10(2)					
1Imd	2.02(2)	1(1)					
1Imd	2.19(2)	0(1)	3(2)	0.0638	733.196	53.755	9
1N/O							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O	2.13(2)	2(1)					
1Br	2.46(3)	9(3)					
1Imd	2.25(9)	2(16)					
1Imd	2.02(3)	3(3)					
1Imd	2.16(6)	3(6)	4(2)	0.1091	1253.837	107.721	11
0N/O							
2Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9

Zn-N(2.0) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(1)	1(1)					
1Br	2.45(2)	9(2)					
1Imd	2.01(2)	0(1)	1(2)	0.0818	940.339	60.125	7
2N/O	2.15(2)	0(1)					
2Br	2.46(3)	13(3)					
1Imd	2.03(3)	0(2)	2(3)	0.1715	1970.536	125.996	7
2N/O	2.13(1)	0(1)					
1Br	2.46(2)	11(2)					
1Imd	2.19(2)	1(1)					
1Imd	2.02(2)	1(1)	3(2)	0.0636	731.093	53.601	9
1N/O			No Fit	No Fit	No Fit	No Fit	9

2Br							
1Imd							
1Imd							
1N/O	2.13(2)	2(1)					
1Br	2.46(3)	9(3)					
1Imd	2.25(0.10)	2(16)					
1Imd	2.16(6)	3(6)					
1Imd	2.02(3)	3(3)	4(2)	0.1091	1253.710	107.710	11
0N/O							
2Br	2.46(3)	14(4)					
1Imd	2.23(4)	5(6)					
1Imd	2.12(5)	5(7)					
1Imd	2.02(4)	3(5)	3(3)	0.2744	3152.497	231.127	9

Zn-N(2.0) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.14(1)	1(1)					
1Br	2.45(2)	9(2)					
1Imd	2.01(2)	0(1)	1(2)	0.0827	949.694	60.723	7
2N/O	2.15(2)	0(1)					
2Br	2.47(3)	14(3)					
1Imd	2.03(3)	0(2)	2(3)	0.1727	1984.662	126.899	7
2N/O	2.13(1)	0(1)					
1Br	2.46(2)	11(2)					
1Imd	2.02(2)	1(1)					
1Imd	2.19(2)	1(1)	3(1)	0.0636	730.345	53.546	9
1N/O							
2Br							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	9
1N/O							
1Br							
1Imd							
1Imd							
1Imd			No Fit	No Fit	No Fit	No Fit	11
0N/O							
2Br	2.46(3)	14(4)					
1Imd	2.23(4)	5(6)					
1Imd	2.12(5)	6(6)					
1Imd	2.02(4)	3(5)	3(3)	0.2743	3151.701	231.069	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.31(1)	0(1)					
1Br	2.24(7)	19(9)					
1Imd	1.96(1)	0(1)	neg5(1)	0.0272	312.837	22.936	9
1N/O	2.07(1)	3(1)					
1S	2.30(2)	0(1)					
1Br	2.14(0.11)	20(17)					
1Imd	1.95(2)	0(1)					
1Imd	2.09(6)	7(9)	neg5(2)	0.0458	525.636	45.159	11

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.31(1)	0(1)					
1Br	2.26(6)	18(8)					
1Imd	1.96(1)	0(1)	neg5(1)	0.0258	296.509	21.739	9
1N/O	2.07(1)	3(1)					
1S	2.30(1)	0(1)					
1Br	2.19(0.12)	22(18)					
1Imd	2.10(5)	5(7)					
1Imd	1.96(2)	0(1)	neg4(2)	0.0453	520.587	44.725	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.31(1)	0(1)					
1Br	2.24(7)	18(9)					
1Imd	1.96(1)	0(1)	neg5(1)	0.0305	350.953	25.730	9
1N/O	2.07(2)	2(1)					
1S	2.30(2)	1(1)					
1Br	2.01(7)	12(5)					
1Imd	1.95(2)	1(1)					
1Imd	1.91(0.12)	12(16)	neg8(3)	0.0494	567.538	48.759	11

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.31(1)	0(1)					
1Br	2.26(6)	17(7)					
1Imd	1.96(1)	0(1)	neg5(1)	0.0289	331.456	24.301	9
1N/O	2.07(1)	3(1)	neg5(2)	0.0514	590.462	50.729	11

1S	2.30(2)	0(1)					
1Br	2.18(0.13)	22(19)					
1Imd	2.09(6)	6(8)					
1Imd	1.96(2)	0(1)					

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.31(1)	0(1)					
1Br	2.24(7)	17(9)					
1Imd	1.95(1)	0(1)	neg6(1)	0.0328	376.797	27.625	9
1N/O	2.10(1)	2(1)					
1S	2.39(6)	2(6)					
1Br	2.39(6)	5(3)					
1Imd	2.14(3)	0(2)					
1Imd	1.98(2)	1(1)	neg2(2)	0.0596	684.344	58.794	11

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1S	2.31(1)	0(1)					
1Br	2.26(6)	16(7)					
1Imd	1.96(1)	0(1)	neg5(1)	0.0309	355.138	26.037	9
1N/O	2.07(1)	3(1)					
1S	2.30(2)	0(1)					
1Br	2.17(0.13)	21(20)					
1Imd	1.95(2)	0(2)					
1Imd	2.09(7)	7(11)	neg6(3)	0.0553	635.830	54.626	11

Zn-N(2.0) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
3N/O	2.09(1)	2(1)					
1S	2.31(1)	2(1)					
1Imd	1.96(1)	2(1)	neg5(1)	0.0319	365.959	23.399	9

Zn-N(2.0) Zn-N(2.2) Zn-S(2.2) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
2N/O	2.08(1)	1(1)					
1N/O	2.20(2)	2(3)					
1S	2.30(1)	3(3)					
1Imd	1.96(1)	0(1)	neg3(1)	0.0254	291.312	21.358	9

1N/O	2.06(2)	2(1)					
2N/O	2.16(2)	1(4)					
1S	2.30(1)	3(3)					
1Imd	1.96(1)	1(1)	neg3(1)	0.0230	264.377	19.383	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(1)	3(1)					
2S	2.33(2)	2(1)					
1Br	2.32(3)	5(2)					
1Imd	1.96(1)	1(1)	neg6(1)	0.0294	337.416	24.738	9

Zn-N(2.0) Zn-S(2.2) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(1)	3(1)					
2S	2.32(2)	2(1)					
1Br	2.32(3)	6(2)					
1Imd	1.96(1)	1(1)	neg6(1)	0.0283	325.338	23.852	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	2(1)					
2S	2.34(2)	2(2)					
1Br	2.33(3)	4(2)					
1Imd	1.96(1)	0(1)	neg6(1)	0.0290	333.240	24.432	9

Zn-N(2.0) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	2(1)					
2S	2.33(2)	3(1)					
1Br	2.33(3)	5(2)					
1Imd	1.96(1)	0(1)	neg7(1)	0.0284	326.512	23.938	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	2(1)					
2S	2.35(2)	3(2)					
1Br	2.34(3)	4(1)					
1Imd	1.95(1)	0(1)	neg7(1)	0.0279	320.206	23.476	9

Zn-N(2.0) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.07(1)	2(1)					
2S	2.34(2)	3(2)					
1Br	2.33(3)	5(1)					
1Imd	1.95(1)	0(1)	neg7(1)	0.0275	316.136	23.178	9

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.42(2)	5(1)					
1S	2.30(1)	4(1)					
1Br	2.36(2)	1(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0133	152.281	13.083	11
1S	2.27(4)	3(3)					
1S	2.36(2)	4(2)					
1Br	2.29(4)	1(2)					
1Imd	2.09(8)	6(13)					
1Imd	1.97(4)	2(4)	neg6(3)	0.0822	943.865	81.091	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.43(2)	4(1)					
1Br	2.37(2)	2(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0120	137.414	11.806	11
1S	2.26(4)	3(3)					
1S	2.36(3)	4(2)					
1Br	2.30(5)	1(3)					
1Imd	1.97(4)	2(4)					
1Imd	2.10(7)	5(11)	neg6(3)	0.0841	966.554	83.040	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.42(2)	4(1)					
1Br	2.37(2)	2(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0112	129.039	11.086	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.3) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(1)	4(1)	neg6(1)	0.0196	224.989	19.330	11

1S	2.28(1)	1(1)					
1S	2.41(3)	5(3)					
1Br	2.76(2)	10(2)					
1Imd	1.96(1)	1(1)					

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.43(2)	4(1)					
1Br	2.37(2)	1(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0116	132.914	11.419	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.43(2)	4(1)					
1Br	2.37(2)	2(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0108	123.594	10.618	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.43(2)	4(1)					
1Br	2.37(2)	2(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0101	115.909	9.958	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.42(2)	4(1)					
1S	2.30(1)	4(1)					
1Br	2.36(2)	2(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0127	146.336	12.572	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(2)	4(1)					
1Br	2.38(2)	1(2)	neg5(1)	0.0104	119.831	10.295	11

1Imd	1.95(1)	1(1)					

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(2)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0097	111.539	9.583	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.44(2)	4(1)					
1Br	2.38(2)	2(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0091	104.749	8.999	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.43(2)	3(1)					
1Br	2.38(2)	2(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0086	98.894	8.496	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.08(1)	3(1)					
1S	2.31(1)	0(1)					
1S	2.49(4)	12(6)					
1Br	2.02(4)	14(4)					
1Imd	1.95(1)	0(1)	neg5(2)	0.0282	323.526	27.795	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0083	95.335	8.191	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	2(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(0)	neg5(1)	0.0078	89.409	7.681	11

Zn-N(2.0) Zn-S(2.2) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	2(1)					
1Imd	1.95(1)	1(0)	neg5(1)	0.0073	84.369	7.248	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.43(2)	4(1)					
1Br	2.37(2)	1(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0116	133.237	11.447	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.43(2)	4(1)					
1Br	2.37(2)	1(2)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0107	122.935	10.562	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.43(2)	4(1)					
1Br	2.37(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0100	114.940	9.875	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.4) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.06(1)	4(1)	neg6(2)	0.0204	234.476	20.145	11

1S	2.28(1)	1(1)					
1S	2.41(3)	5(3)					
1Br	2.76(2)	10(2)					
1Imd	1.96(1)	1(2)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(2)	4(1)					
1Br	2.38(2)	0(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0104	119.483	10.265	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0096	110.313	9.477	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0090	103.278	8.873	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.30(1)	3(1)					
1S	2.43(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0085	97.403	8.368	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	0(1)	neg5(1)	0.0090	103.870	8.924	11

1Imd	1.95(1)	1(1)					

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(1)	4(2)					
1Br	2.38(2)	0(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0083	95.481	8.203	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(0)	neg5(1)	0.0078	89.365	7.678	11

Zn-N(2.0) Zn-S(2.3) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(1)	1(1)					
1Imd	1.95(1)	1(0)	neg5(1)	0.0073	84.406	7.252	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(2)	4(1)					
1Br	2.38(2)	0(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0110	126.941	10.906	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.44(2)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0102	117.136	10.064	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.43(2)	4(1)					
1S	2.31(1)	3(1)					
1Br	2.37(2)	1(2)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0119	136.679	11.743	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.5) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.43(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg5(1)	0.0091	104.149	8.948	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	0(1)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0096	110.325	9.478	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	0(1)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0088	101.250	8.699	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0083	95.021	8.164	11

Zn-N(2.0) Zn-S(2.4) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)	neg6(1)	0.0079	90.211	7.750	11

1S	2.31(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(0)					

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.3) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.44(2)	4(1)					
1S	2.32(1)	2(1)					
1Br	2.38(2)	0(2)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0126	144.654	12.428	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.4) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	2(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	0(1)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0095	108.971	9.362	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.5) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.31(1)	3(1)					
1S	2.44(1)	4(1)					
1Br	2.38(2)	0(1)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0089	102.291	8.788	11

Zn-N(2.0) Zn-S(2.5) Zn-S(2.6) Zn-Br(2.6) Zn-Imd

N	Radius Å	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Red χ^2	nvar
1N/O	2.05(1)	5(1)					
1S	2.44(2)	4(1)					
1S	2.31(1)	3(1)					
1Br	2.38(2)	1(1)					
1Imd	1.95(1)	1(1)	neg6(1)	0.0106	121.737	10.459	11

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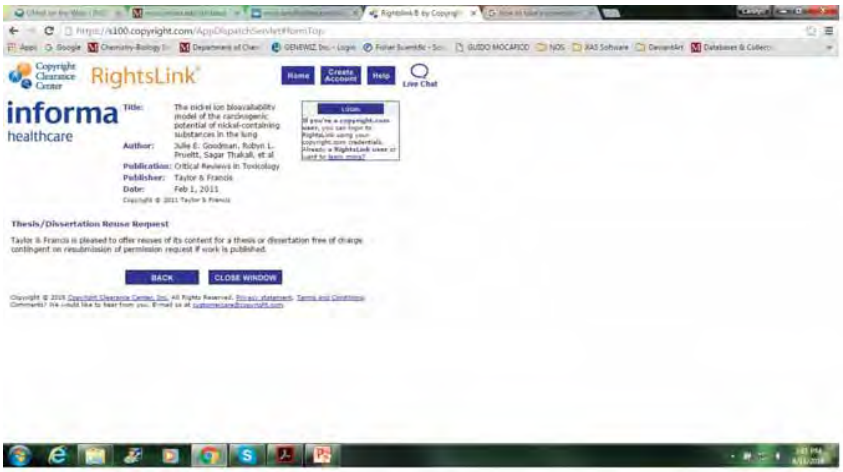
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Author:
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Publication:
Critical Reviews in Toxicology
Publisher:
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